

The NBO Pattern in Luminescent Chromophores: Unravelling Excited-State Features with TD-DFT

Supporting Information

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1. Additional methodological testing

1.a. Comparisons between M06-2X and ω B97X-D values

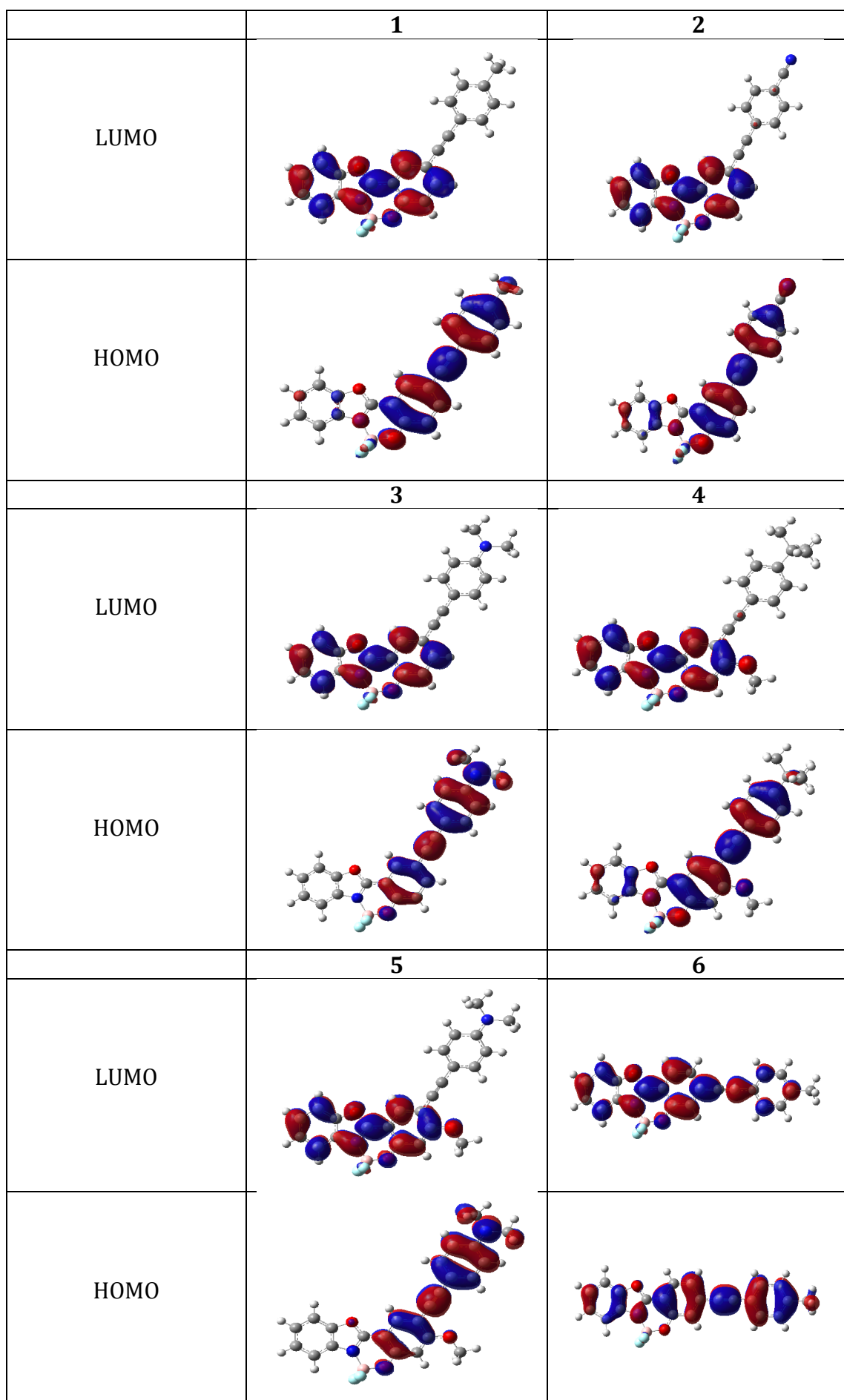
Table S-1: Computed (SS,neq) wavelengths for the first two compounds using two functionals


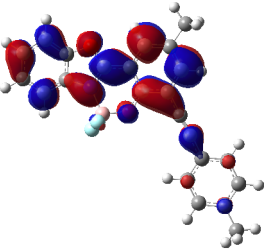
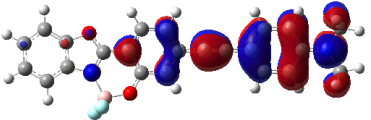
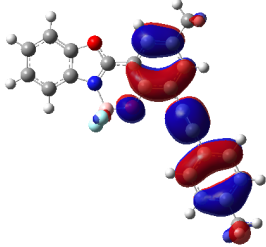
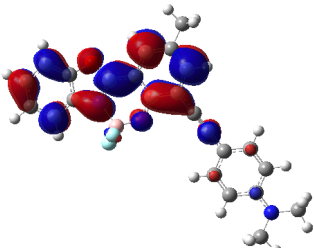
Compound	M06-2X	ω B97X-D
1	347 nm	337 nm
	275 nm	276 nm
2	327 nm	324 nm
	300 nm	296 nm

Table S-2: Computed ω B97X-D wavelengths for compound 1 using several atomic basis sets. All calculations on the ω B97X-D/6-31G(d) geometry with the PCM model in toluene.

Basis set	(LR,eq)
6-31G(d)	332 nm
6-31+G(d)	335 nm
6-311G(d,p)	335 nm
6-311++G(d,p)	338 nm
6-311+G(2d,p)	339 nm

2. Representation of frontier MO for dyes 1-9



	7	8
LUMO		
HOMO		
	9	
LUMO		
HOMO	