-Supplementary Information-

Sulphur- and Selenium-for-Oxygen Replacement as a Strategy to Obtain Dual TypeI/TypeII Photosensitizers for Photodynamic Therapy

Mario Prejanò , Marta Erminia Alberto * , Bruna Clara De Simone, Tiziana Marino , Marirosa Toscano and Nino Russo *

Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, 87036 Arcavacata di Rende, CS, Italy.

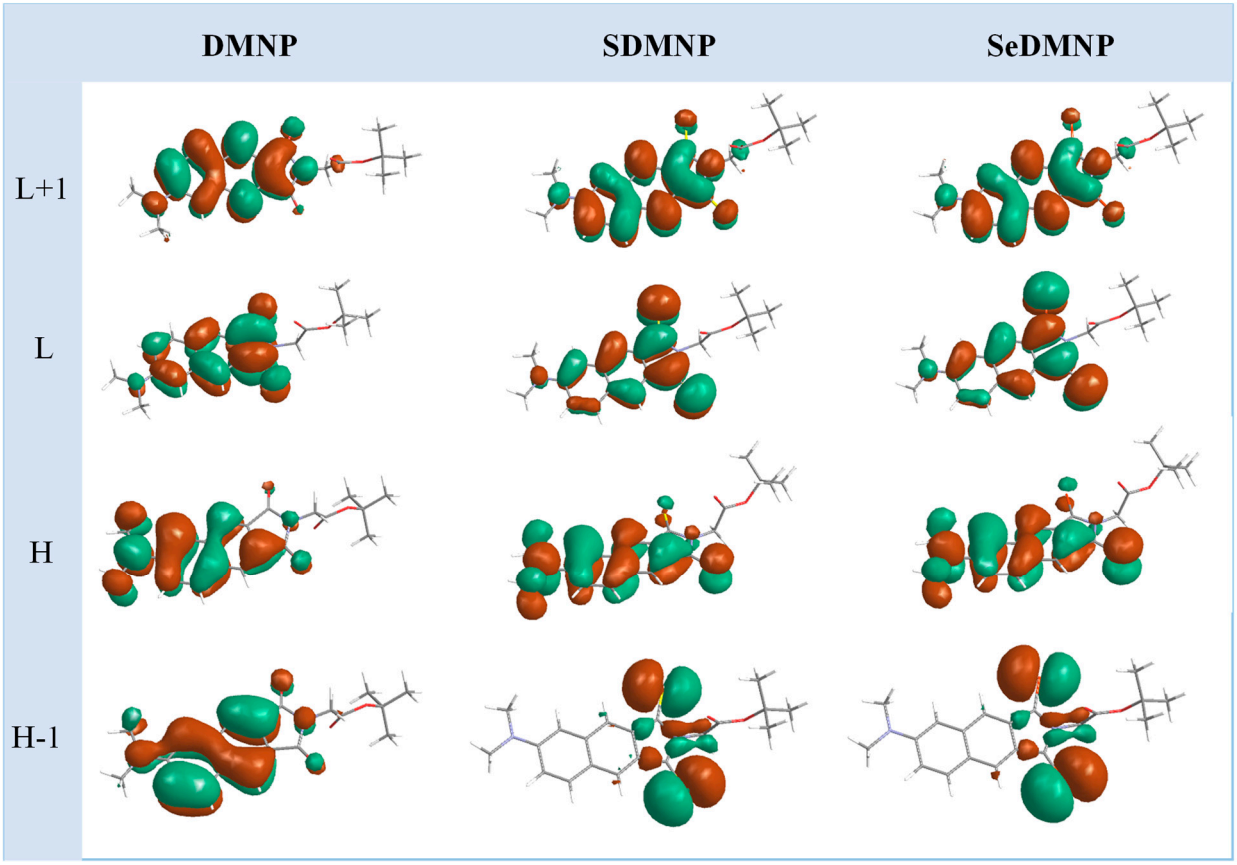
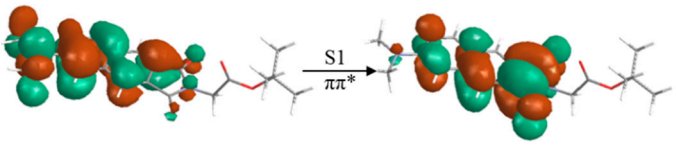
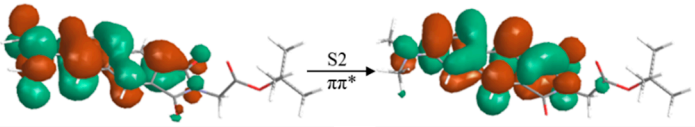
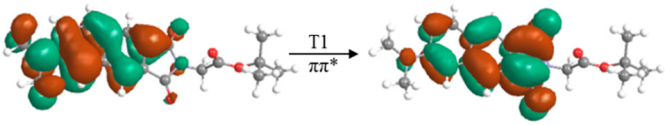
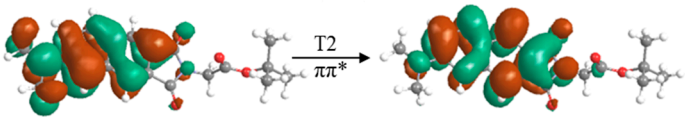
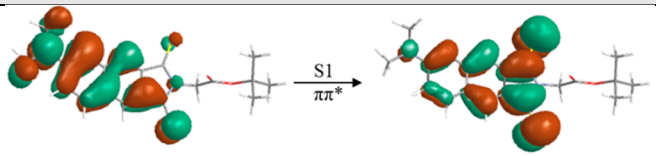
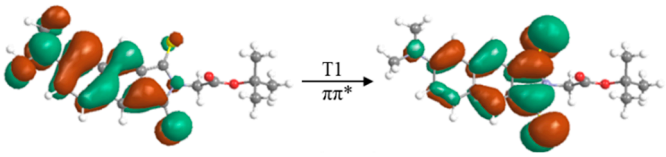
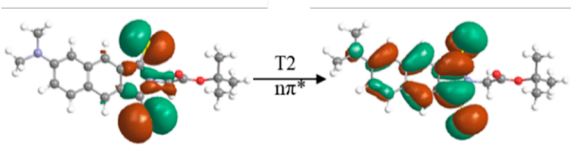


Figure S1: Frontiers Molecular Orbital Plots

State	Composition	λ	ΔE	f	Natural Transition Orbitals (NTOs)
DMNP					
S_1	H→L	449	2.76	0.135	
S_2	H→L+1	388	3.20	0.304	
T_1	H→L	548	2.26	/	
T2	H-1→L	493	2.51	/	
SDMNP					
S_1	H→L	603	2.05	0.303	
T_1	H→L	867	1.43	/	
T2	H-1→L	626	1.98	/	
SeDMNP					

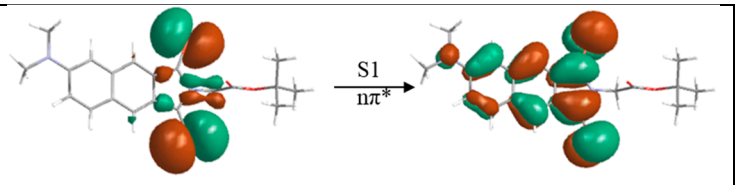
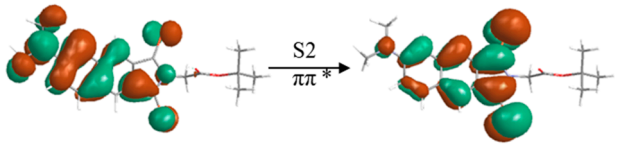
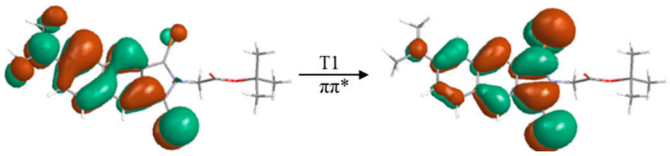
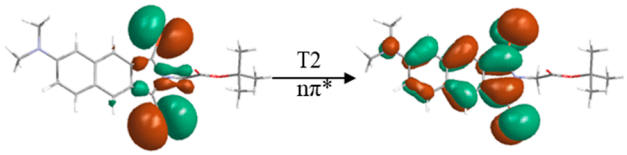
S_1	H-1→L	682	1.82	0.000	
S2	H→L	645	1.92	0.333	
T_1	H→L	1001	1.24	/	
T2	H-1→L	787	1.58	/	

Figure S2: Main Vertical singlet and triplet excitation energies, λ (nm), ΔE (eV), oscillator strength f and Natural Transition Orbitals involved, for DMNP, SDMNP and SeDMNP in DMSO at TD-DFT/B3LYP/6-31+G(d,p) level of theory.

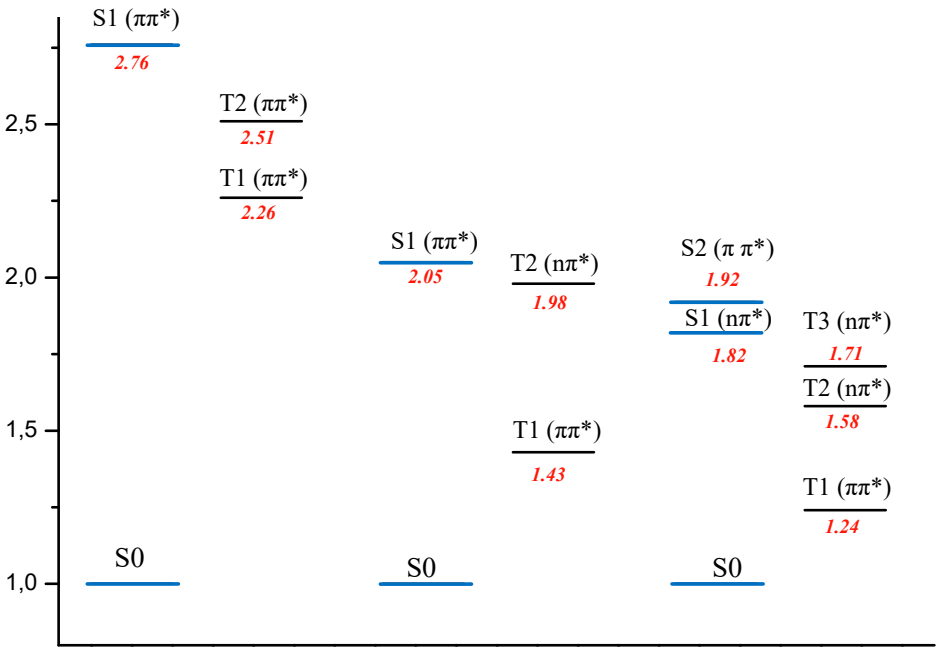


Figure S3. Energy diagram of the main singlet and triplet states.