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Supplementary Information

Excitation energies, singlet-triplet energy gap, spin-orbit matrix elements and heavy atom effect in BOIMPYs as possible photosensitizers in photodynamic therapy. A computational investigation

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Average squared values (cm⁻¹) of Spin-orbit Cartesian components between low-lying singlet and triplet states calculated employing B3LYP in conjunction with different basis sets on 1 and 4 optimized structures at B3LYP/6-31G* level of theory.

Cmpd	Basis set	$\langle \Psi_{S_1} \hat{H}_{so} \Psi$	$Y_{T_1} \langle \Psi_{S_1} \hat{H}_{so} \rangle$	$\Psi_{T_2} \langle \Psi_{S_1} $	\hat{H}_{so}	$\Psi_{T_3} \Delta E_{S1 \to T1}$	$\Delta E_{S1 \to T2}$	$\Delta E_{S1 \to T3}$
1	cc-pVDZ	0.01	0.28	2 1		1.40	0.36	
	cc-pVTZ	0.01	0.32			1.39	0.35	
4	cc-pVDZ	5.31	44.56	3	1.26	1.30	0.31	0.20
	cc-pVTZ	5.41	41.43	3	1.68	1.28	0.30	0.17

-Figure S1-

