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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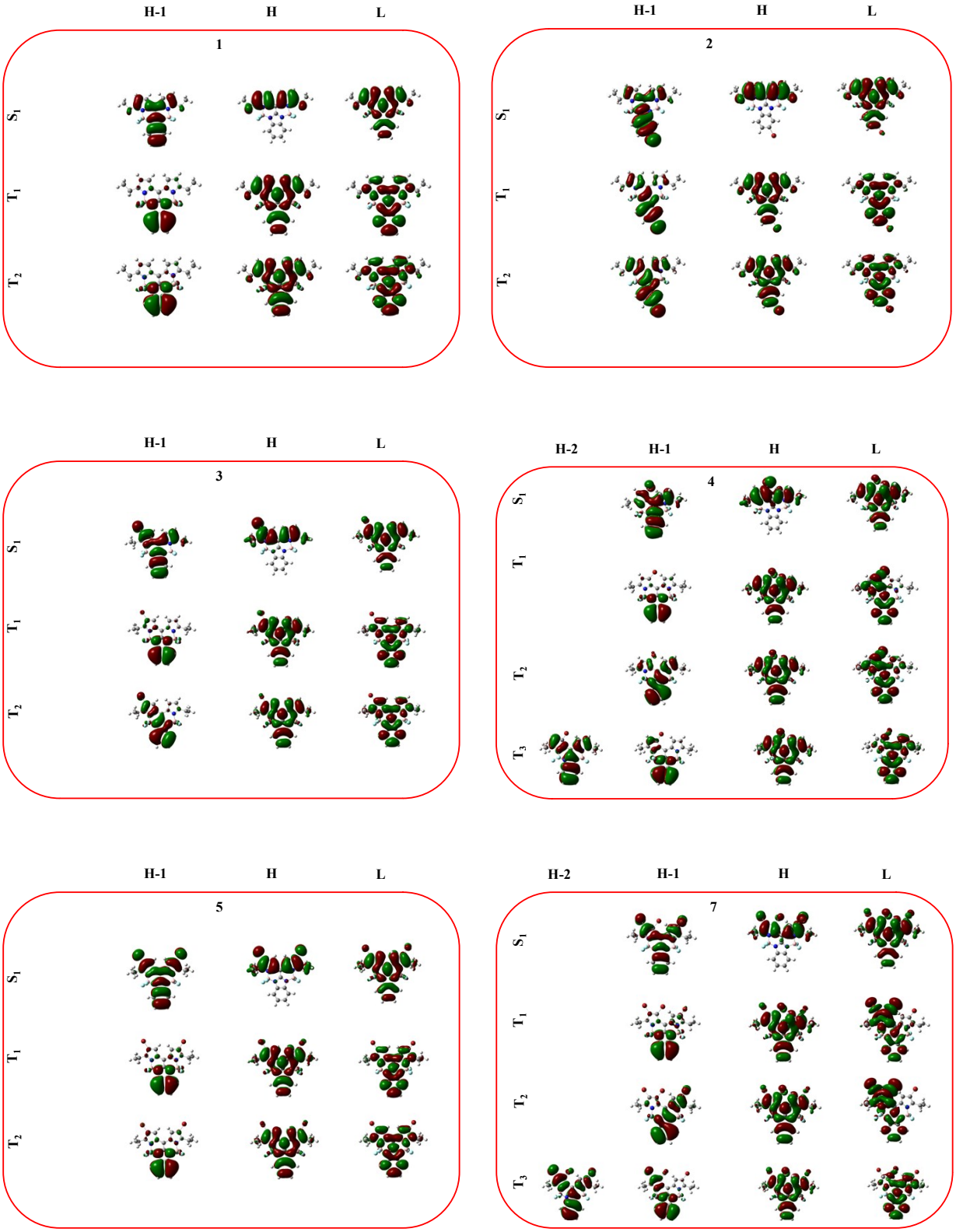
Table of Contents

-Table S1-

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	$\langle\Psi_{S_1}\lvert\hat{H}_{so}\rvert\Psi_{T_1}$	$\langle\Psi_{S_1}\lvert\hat{H}_{so}\rvert\Psi_{T_2}$	$\langle\Psi_{S_1}\lvert\hat{H}_{so}\rvert\Psi_{T_3}$	$\Delta E_{S1\rightarrow T1}$	$\Delta E_{S1\rightarrow T2}$	$\Delta E_{S1\rightarrow T3}$
1	cc-pVDZ	0.01	0.28		1.40	0.36	
	cc-pVTZ	0.01	0.32		1.39	0.35	
4	cc-pVDZ	5.31	44.56	31.26	1.30	0.31	0.20
	cc-pVTZ	5.41	41.43	31.68	1.28	0.30	0.17

-Figure S1-


H-1
H
L
1
S1
T1
T2
H-1
H
L
2
S1
T1
T2
H-1
H
L
3
S1
T1
T2
H-2
H-1
H
L
4
S1
T1
T2
T3
H-1
H
L
5
S1
T1
T2
H-2
H-1
H
L
7
S1
T1
T2
T3