

## **Molecular design of the organic sensitizers absorbing in broadened visible region for dye-sensitized solar cell**

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Table S1. The frontier molecular orbitals for XS54.

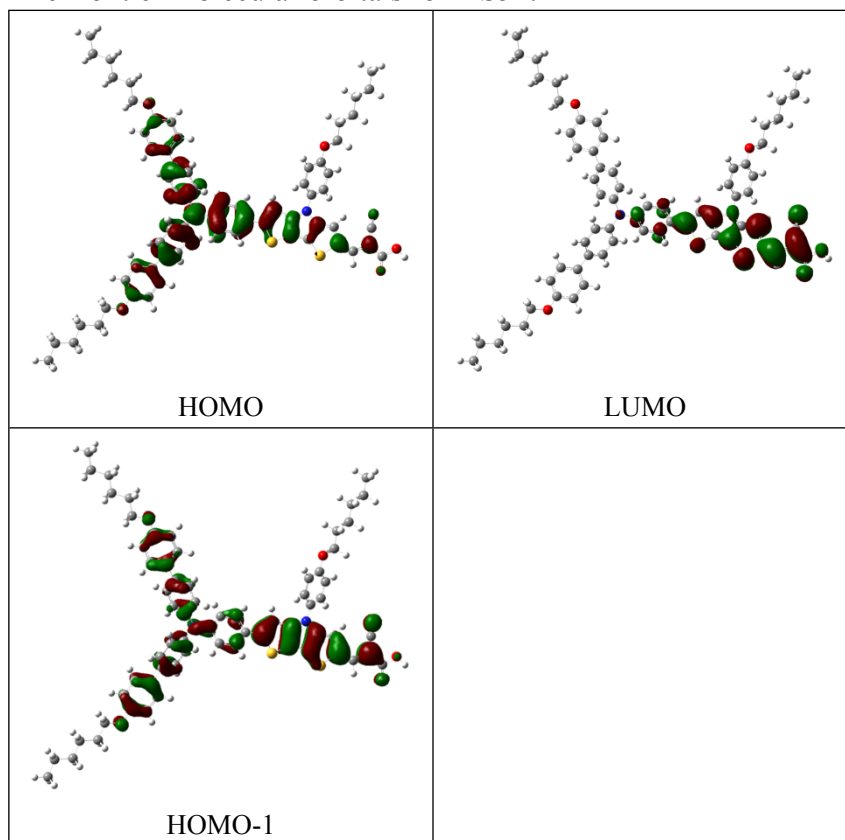
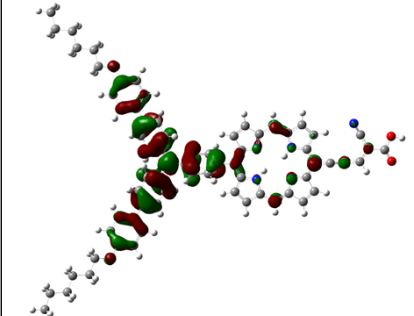
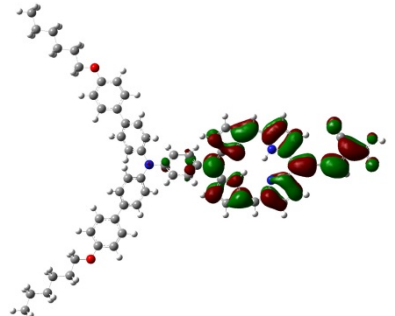
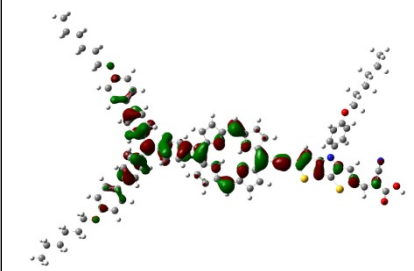
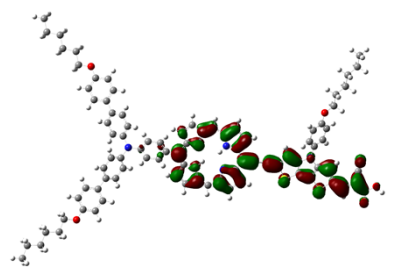
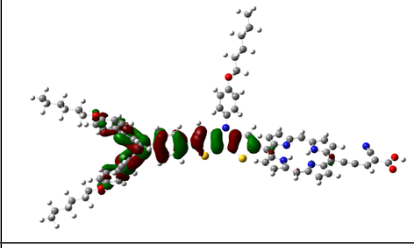
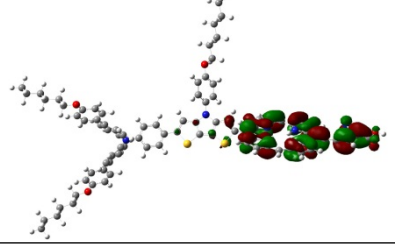
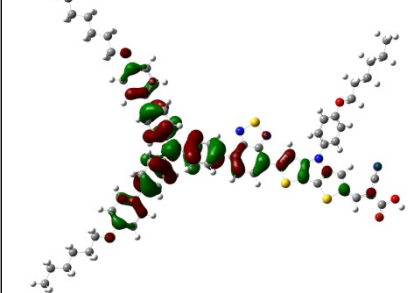
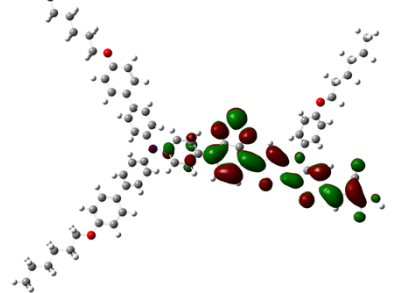

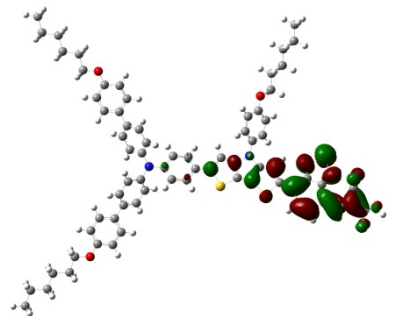


Table S2. The frontier orbitals for the designed molecules.

	HOMO	LUMO
P1		
P2		
P3		
P4		
P5		

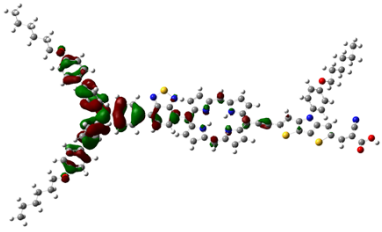
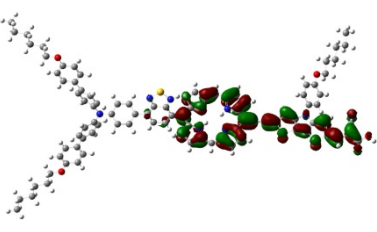

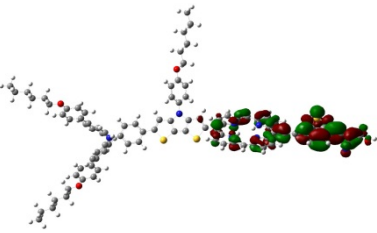
P6	 A ball-and-stick model of a protein-ligand complex. The protein backbone is shown in grey, with side chains in various colors (red, green, blue, yellow). The ligand is a large, multi-ring system with red and green atoms, positioned in the center of the protein's binding pocket.	 A ball-and-stick model of the same protein-ligand complex as in the left panel, but viewed from a different angle. The protein backbone is grey, and the ligand is the red and green multi-ring system.
P7	 A ball-and-stick model of a protein-ligand complex. The protein backbone is grey, and the ligand is a red and green multi-ring system. The view is from a top-down perspective.	 A ball-and-stick model of the same protein-ligand complex as in the left panel, but viewed from a different angle. The protein backbone is grey, and the ligand is the red and green multi-ring system.

Figure S1. The spectrum of XS54 calculated with different functionals compared with the experimental data. The experimental data are taken from Chem. Commun., 49 (2013) 5748-5750.

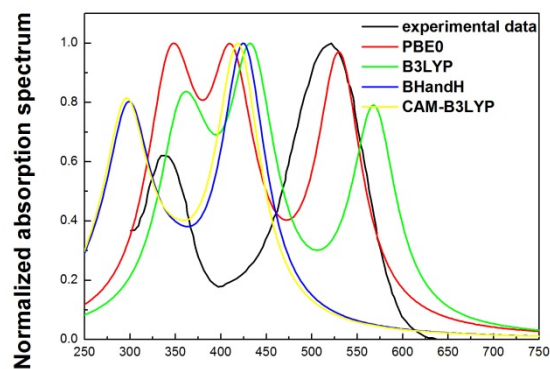


Figure S2. The energy levels of the designed sensitizers and XS54.

