

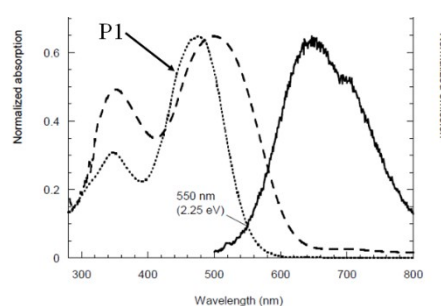
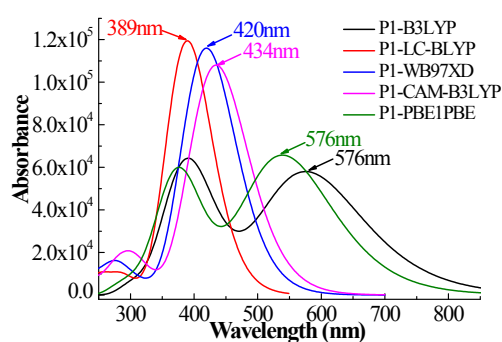
Supporting information

Design of high performance *p*-type sensitizers with pyridinium derivatives as acceptor by theoretical calculations

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Absorption (dotted line) and emission (solid line) spectra of **P1** in MeCN.

Fig. S1 The simulated UV-vis absorption spectrum of **P1** by different functionals using the same basis set 6-311G**, as well as its experimental spectrum

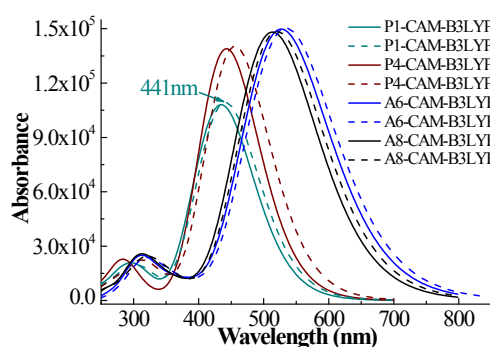


Fig. S2 The simulated UV-vis absorption spectra for some selected dyes at CAM-B3LYP/6-311++G** level