

SUPPORTING MATERIAL

COMPUTATIONAL STUDY OF KHELLIN EXCITED STATES AND PHOTOBINDING TO DNA

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Figure S1. Energy curves for ground and first excited singlet states for Khellin addition to thymine at (a) Pyrone side, (b) furan side. Plots shown for B3LYP and MPWB1K functionals, using the 6-31G(d,p) basis set; all calculations single point TD-DFT based on B3LYP optimized geometries as outlined in text.

