Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

π-conjugation effects on excited-state intermolecular proton transfer reactions in anthracene-urea derivatives in the presence of acetate anions

Atsushi Tachibanaki, Toru Matsui and Yoshinobu Nishimura*

Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1

Tennoudai, Tsukuba, Ibaraki 305-8571, Japan

*Corresponding author e-mail: nishimura@chem.tsukuba.ac.jp (Yoshinobu Nishimura)

1. [1]NMR spectra

2BpUA

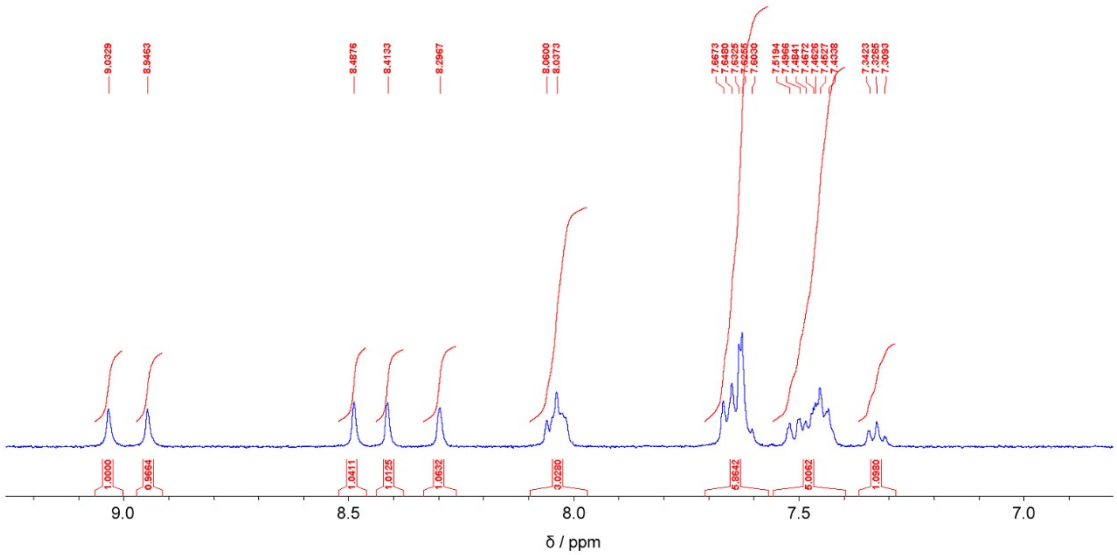

Figure S1. [1]H NMR spectrum of 2BpUA in DMSO-d_6.

2NpUA

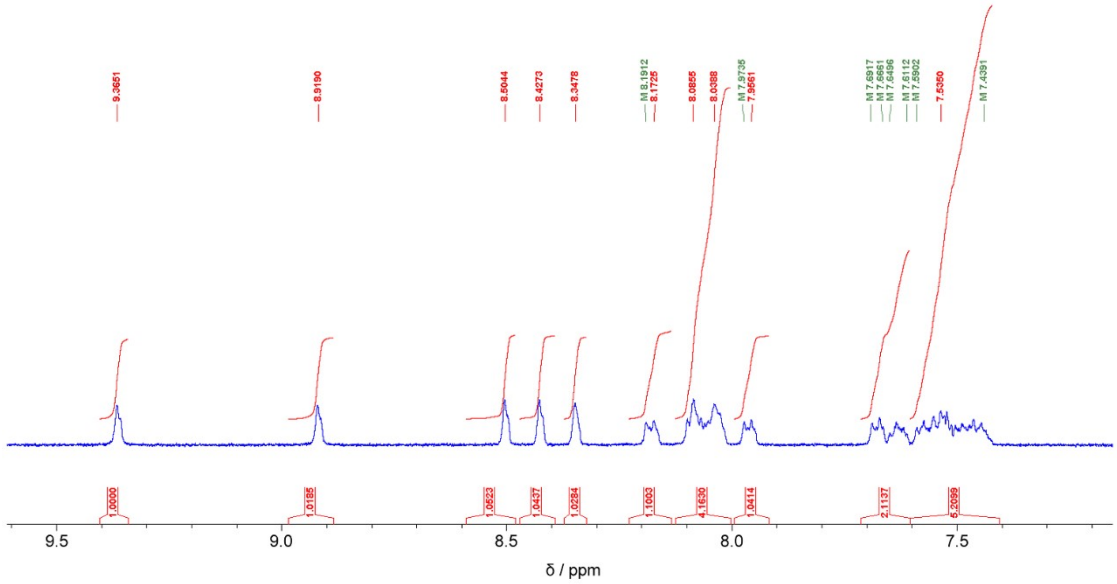

Figure S2. ^{1}H NMR spectrum of 2NpUA in DMSO-d_6.

2BnUA

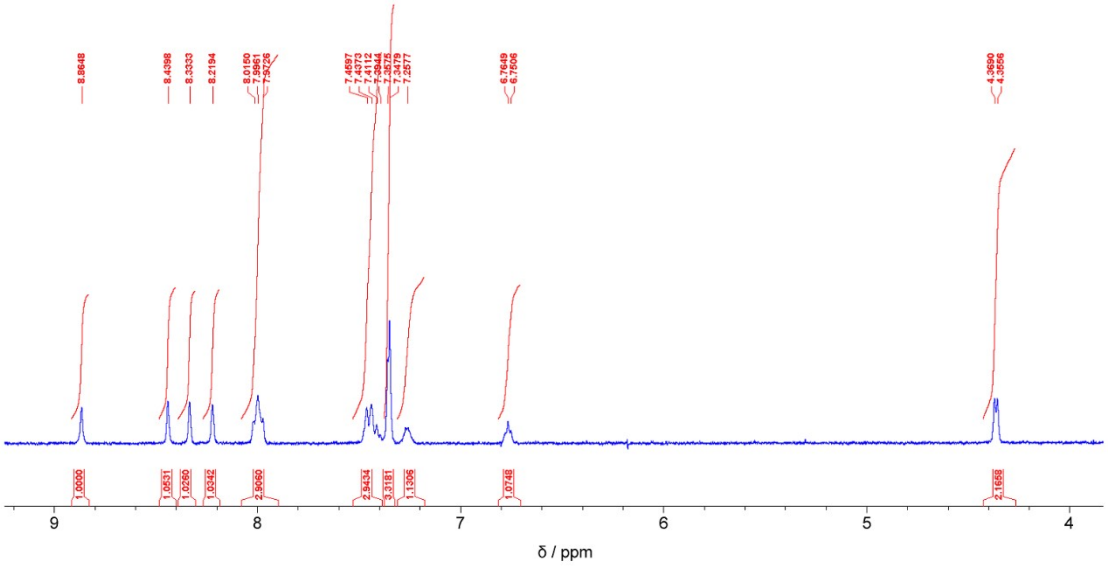

Figure S3. ^{1}H NMR spectrum of 2BnUA in DMSO-d_6.

2CyUA

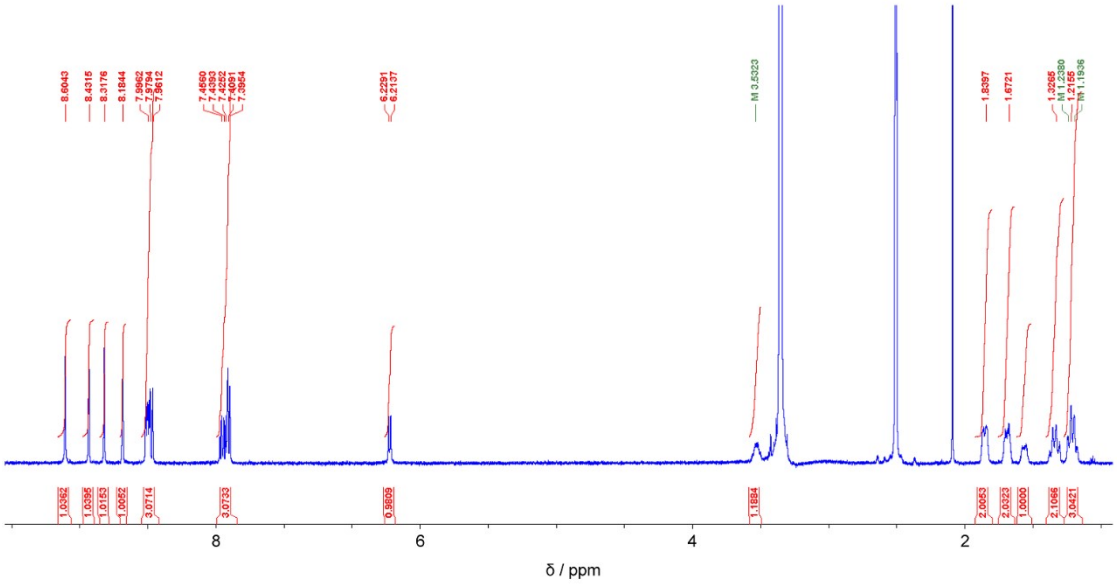

Figure S4. ^{1}H NMR spectrum of 2CyUA in DMSO-d_6.

2. Spectral separation of T* emission

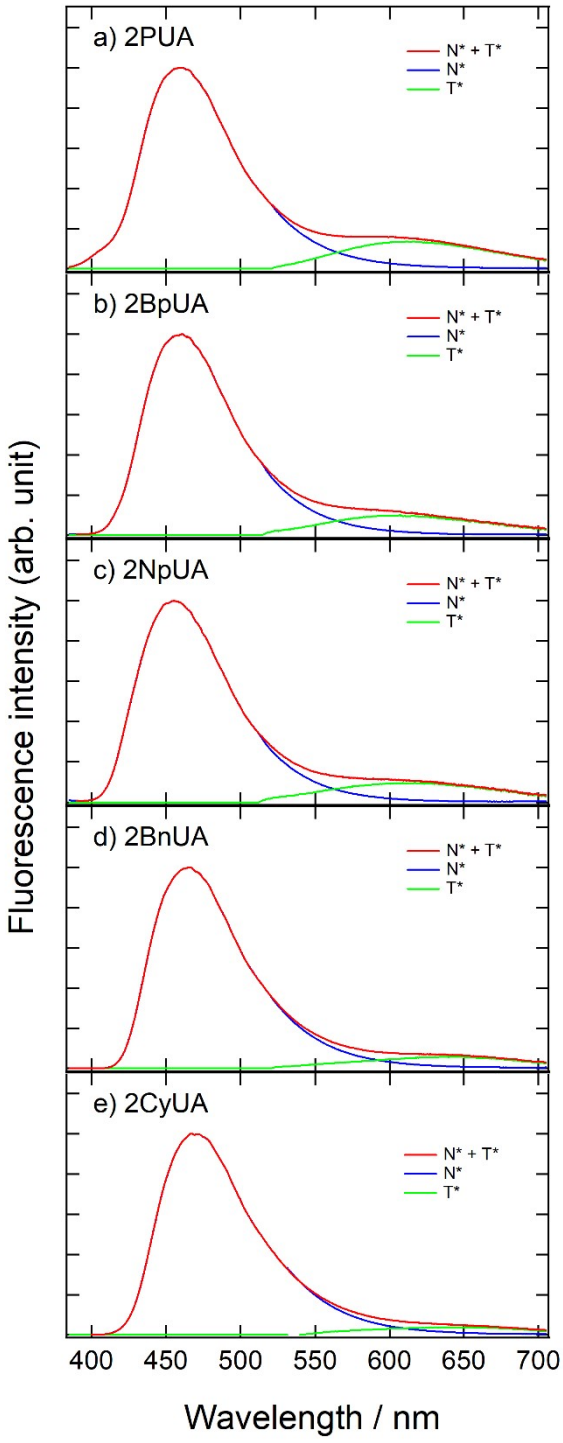

Figure S5. Separated fluorescence spectra of (a) 2PUA, (b) 2BpUA, (c) 2NpUA, (d) 2BnUA and (e) 2CyUA in the presence of TBAAc on excitation at 375 nm in DMSO.

3. Fluorescence lifetimes of 2PUA derivatives

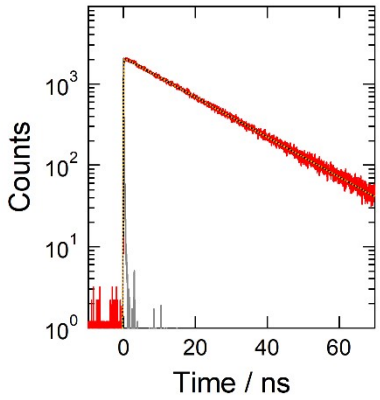

Figure S6. A fluorescence decay curve of 2BpUA observed at 460 nm on excitation at 375 nm in the absence of TBAAc in DMSO.

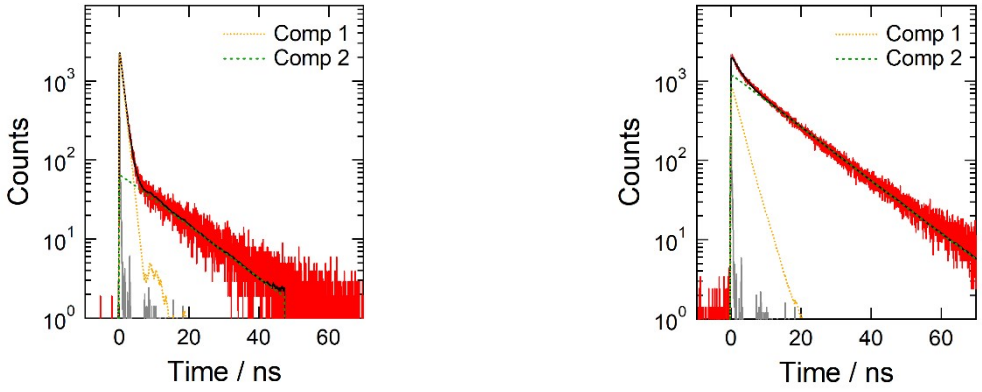

Figure S7. Fluorescence decay curves of 2BpUA observed 460 nm (left) and 640 nm (right) on excitation at 375 nm in the presence of 10 mM TBAAc.

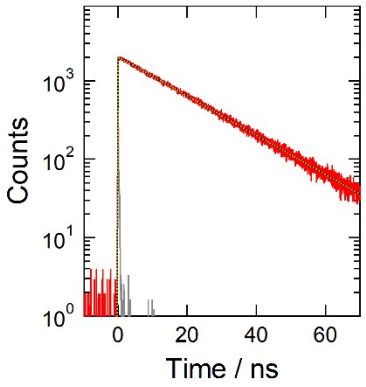

Figure S8. A fluorescence decay curve of 2NpUA observed at 460 nm on excitation at 375 nm in the absence of TBAAc in DMSO.

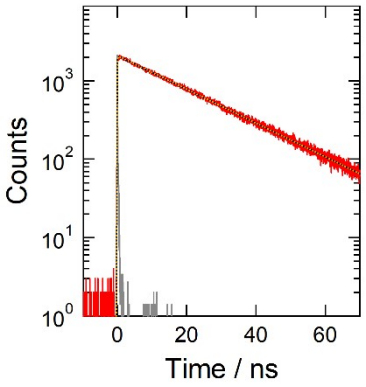

Figure S9. A fluorescence decay curve of 2BnUA observed at 460 nm on excitation at 375 nm in the absence of TBAAc in DMSO.

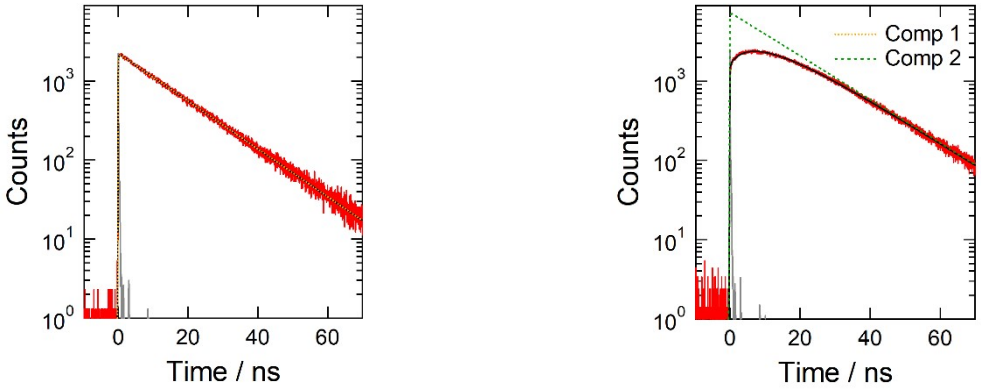

Figure S10. Fluorescence decay curves of 2BnUA observed 460 nm (left) and 640 nm (right) on excitation at 375 nm in the presence of 50mM TBAAc.

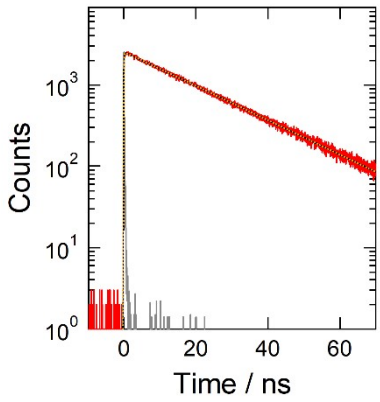

Figure S11. A fluorescence decay curve of 2CyUA observed at 450 nm on excitation at 375 nm in the absence of TBAAc in DMSO.

4. Time-resolved fluorescence spectra of 2PUA derivatives in the presence of TBAAc

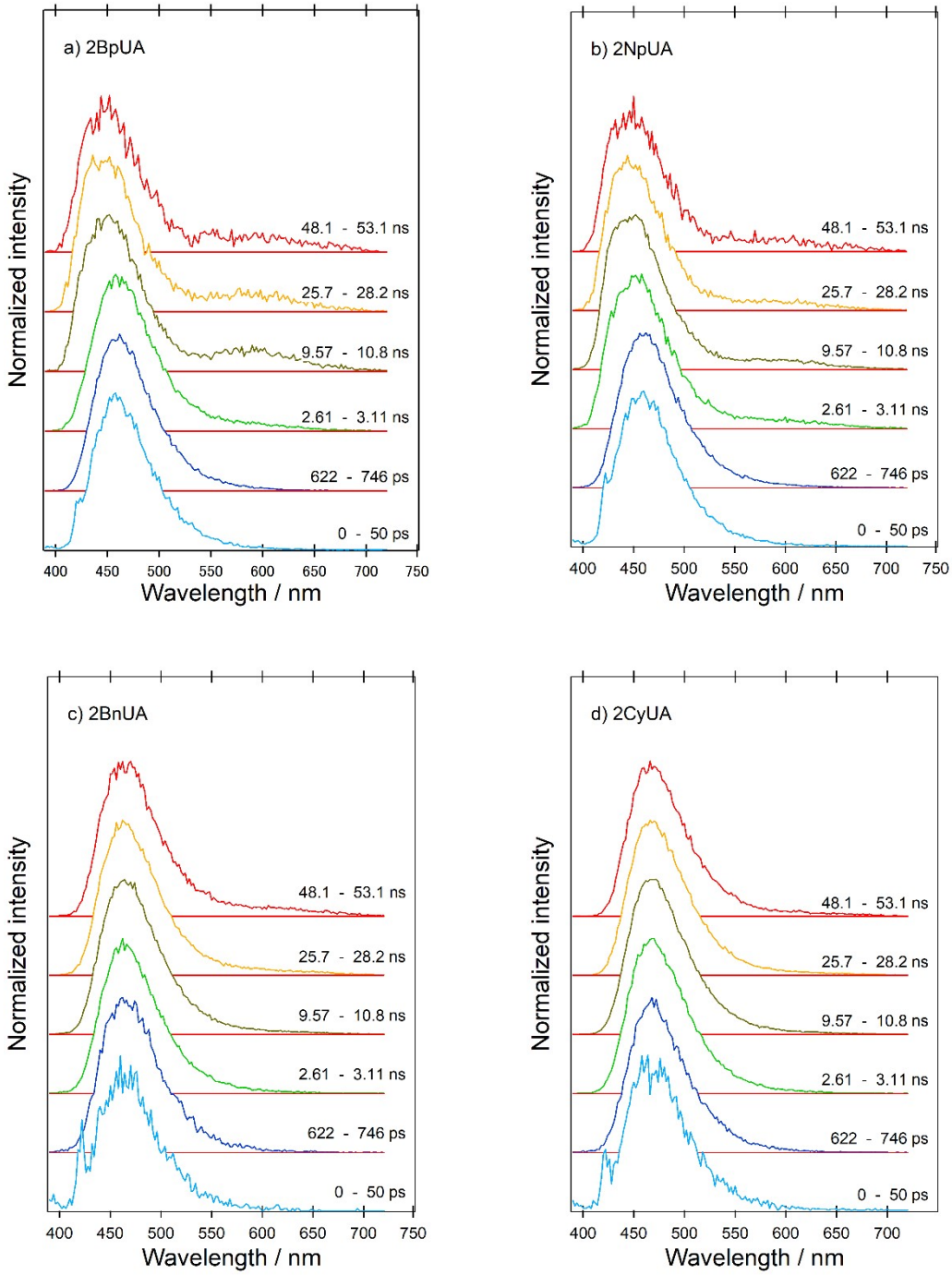

Figure S12. Time-resolved fluorescence spectra of (a) 2BpUA (b) 2NpUA, (c) 2BnUA and (d) 2CyUA excited at 375 nm in the presence of TBAAc in DMSO under Ar.

5. DFT calculations

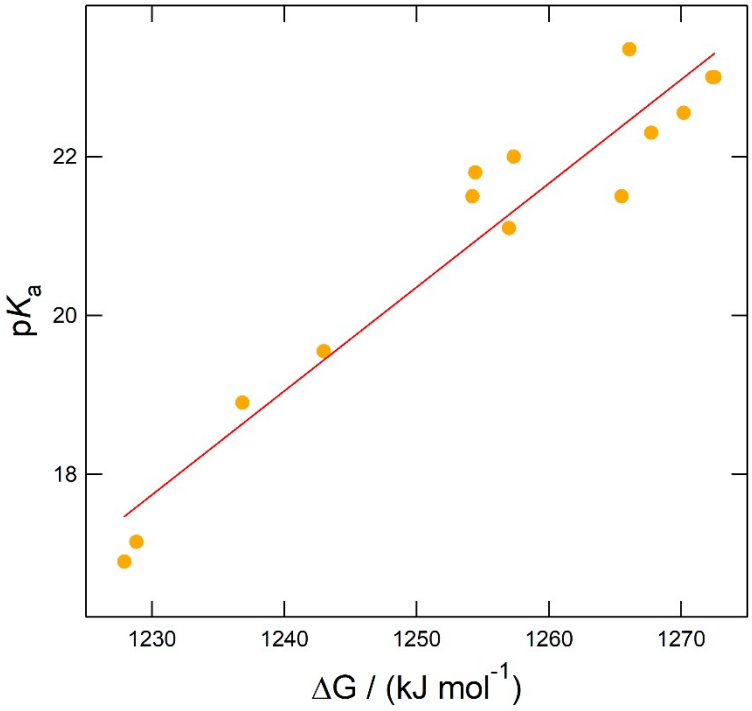

Figure S13. Plots of pK_a vs ΔG.

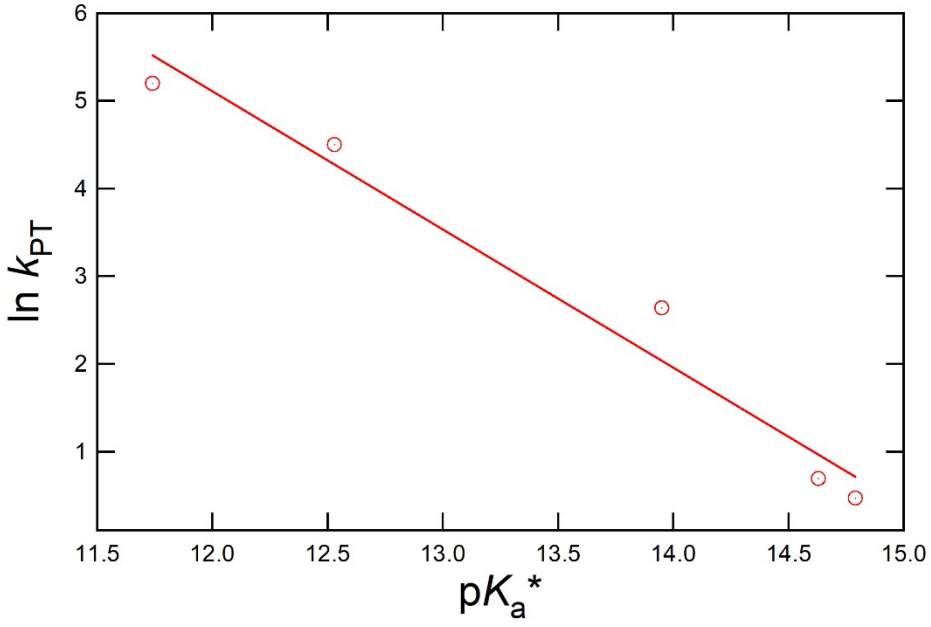

Figure S14. Plots of ln k_{PT} vs pK_a*.