Supporting Information

for

Interactions between photoacidic 3-hydroxy-naphtho[1,2-*b*]quinolizinium and cucurbit[7]uril: Influence on acidity in the ground and excited state

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NMR spectra of compounds 2 and 5; fluorimetric titrations of 2 with acid and CB[7]; determination of 0-0 transition energies; analysis of binding isotherms from photometric titrations of 2 with CB[7]

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1 Additional spectroscopic data

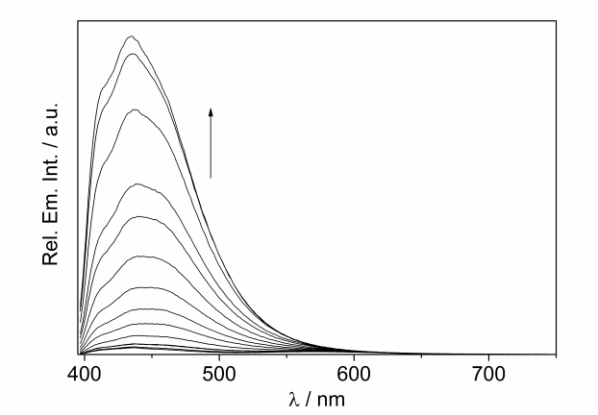

Figure S1: Spectrofluorimetric titration of **2** (c = 10 µM in H_2O) with aq $HClO_4$ (70%); λ_{ex} = 380 nm. The arrow indicates the changes of the spectrum upon successive addition of $HClO_4$.

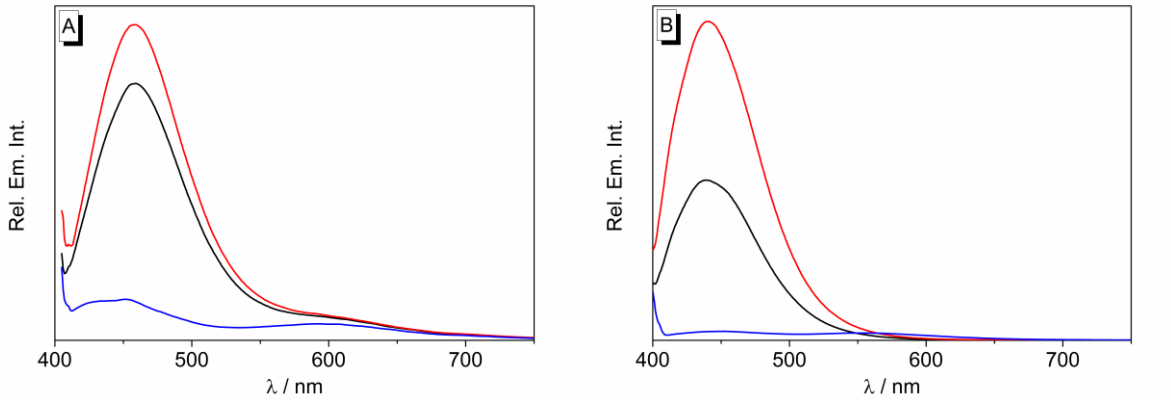

Figure S2: Emission spectra of **2** (c_L = 10 µM) in MeOH (A, λ_{ex} = 400 nm) and MeCN (B, λ_{ex} = 398 nm). Black lines: without addition, red: upon addition of CF_3COOH, blue: upon addition of DBU.

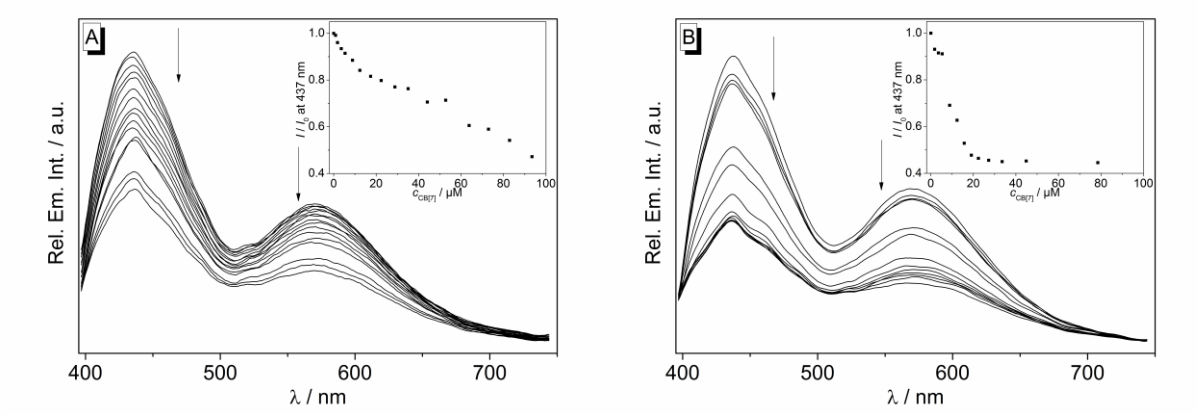

Figure S3: Spectrofluorimetric titration (λ_{ex} = 380 nm) of CB[7] (*c* = 453 µM) to naphthoquinolizinium **2** (*c* = 15 µM) in BPE buffer (with 10% v/v DMSO) at pH 5 (A) und pH 7 (A). Arrows indicate the development of bands with increasing concentration of CB[7]. Insets: Plot of relative emission, I/I_0, at λ = 437 nm versus concentration of CB[7].

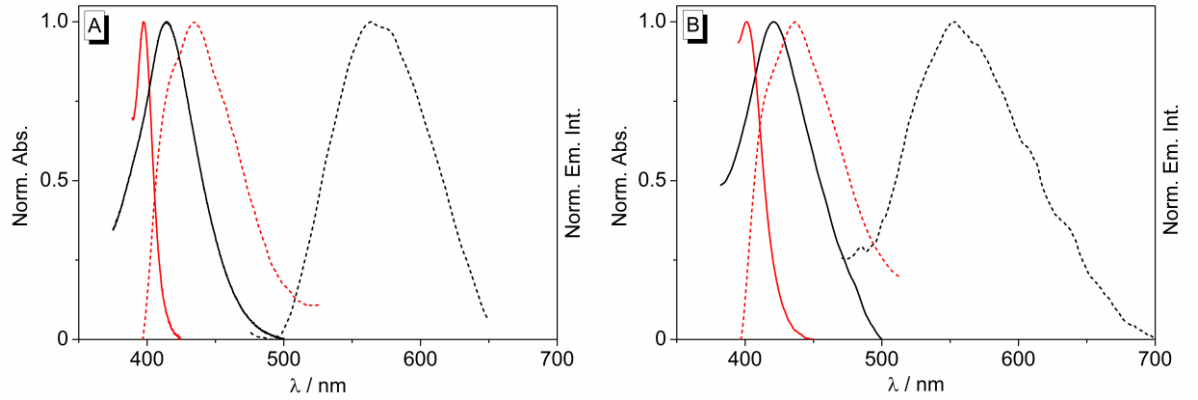

Figure S4: Normalized absorption (continuous lines) and emission bands (dashed lines) of naphthoquinolizinium **2** (*c* = 15 µM) in the absence (A) and in the presence (B) of CB[7] ($c_{CB[7]}$ = 100 µM); red: major band under acidic conditions, black: major band under alkaline conditions.

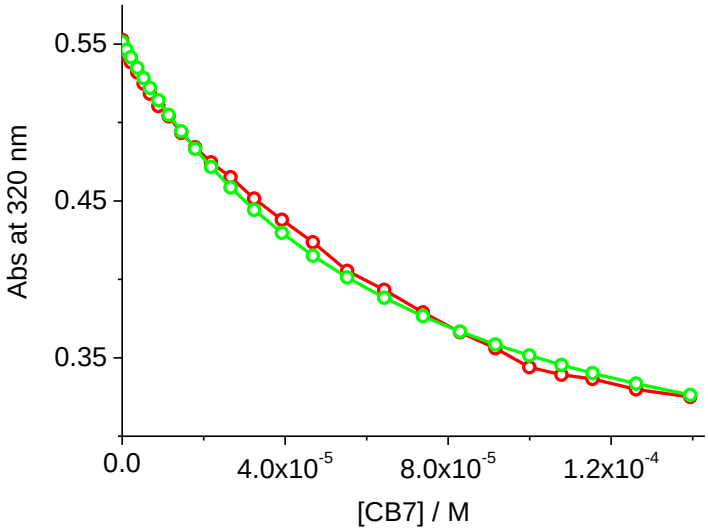

Figure S5: Binding isotherms, i.e. plot of absorption of **2** at λ = 320 nm versus $c_{CB[7]}$ obtained from photometric titration of **2** with CB[7] at pH 5; red = experimental data, green: fit to the theoretical model.

2 ^{1}H NMR and ^{13}C NMR spectra of derivatives 2 and 5

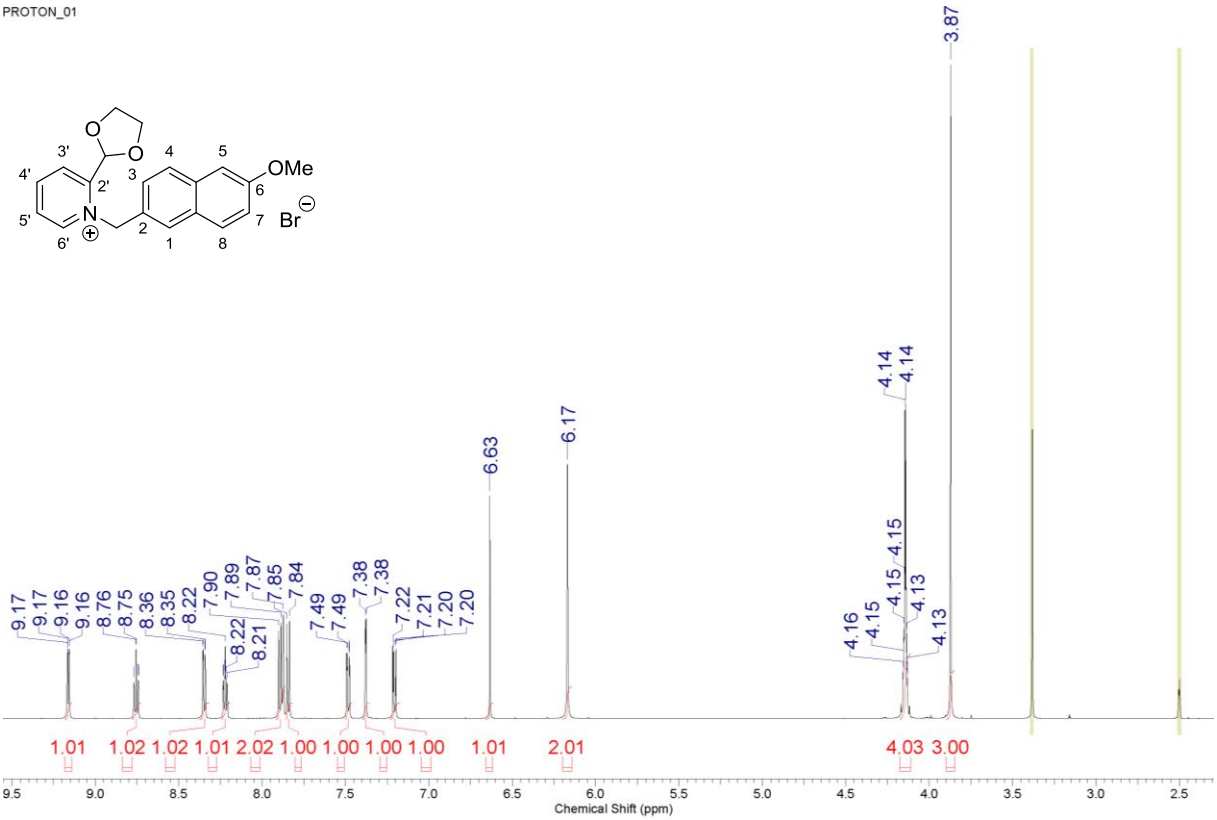

Figure S6: ^{1}H NMR spectrum of 2-(1,3-dioxolan-2-yl)-1-[(6-methoxynaphth-2-yl)methyl]pyridinium bromide (**5**).

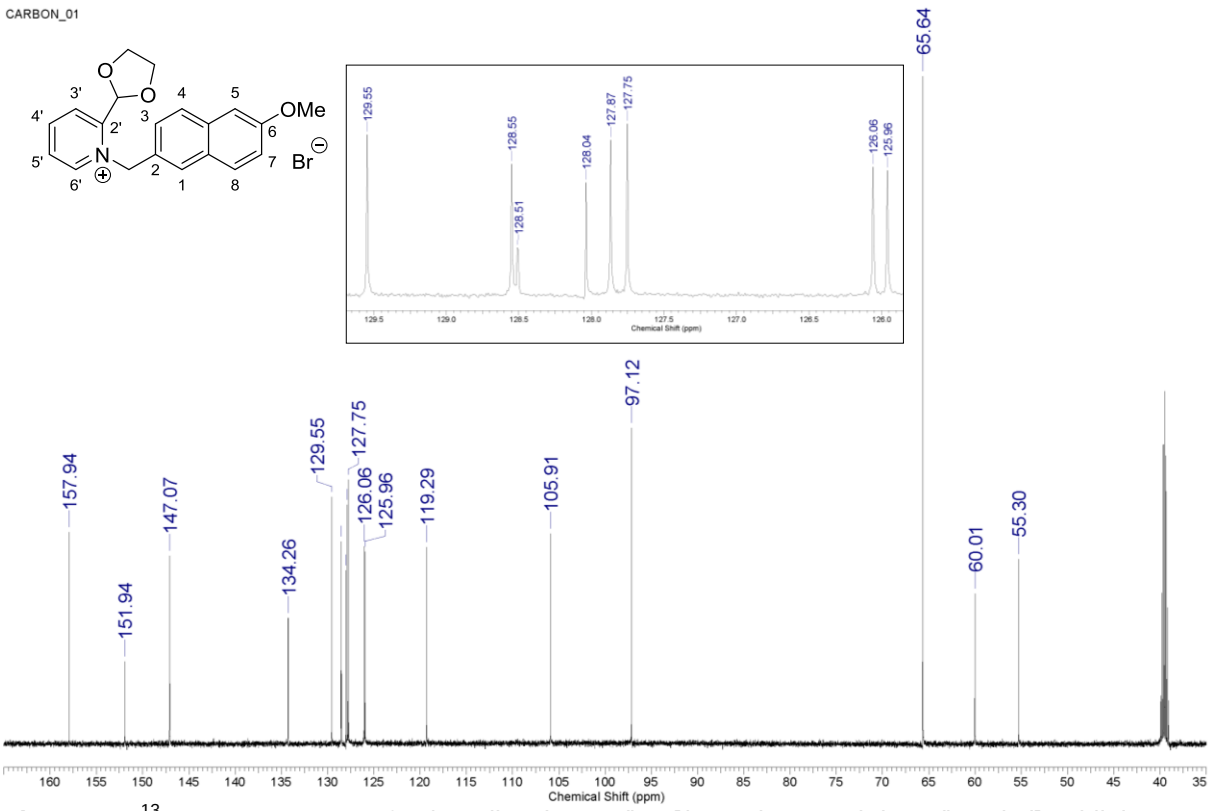

Figure S7: ^{13}C NMR spectrum of 2-(1,3-dioxolan-2-yl)-1-[(6-methoxynaphth-2-yl)methyl]pyridinium bromide (**5**).

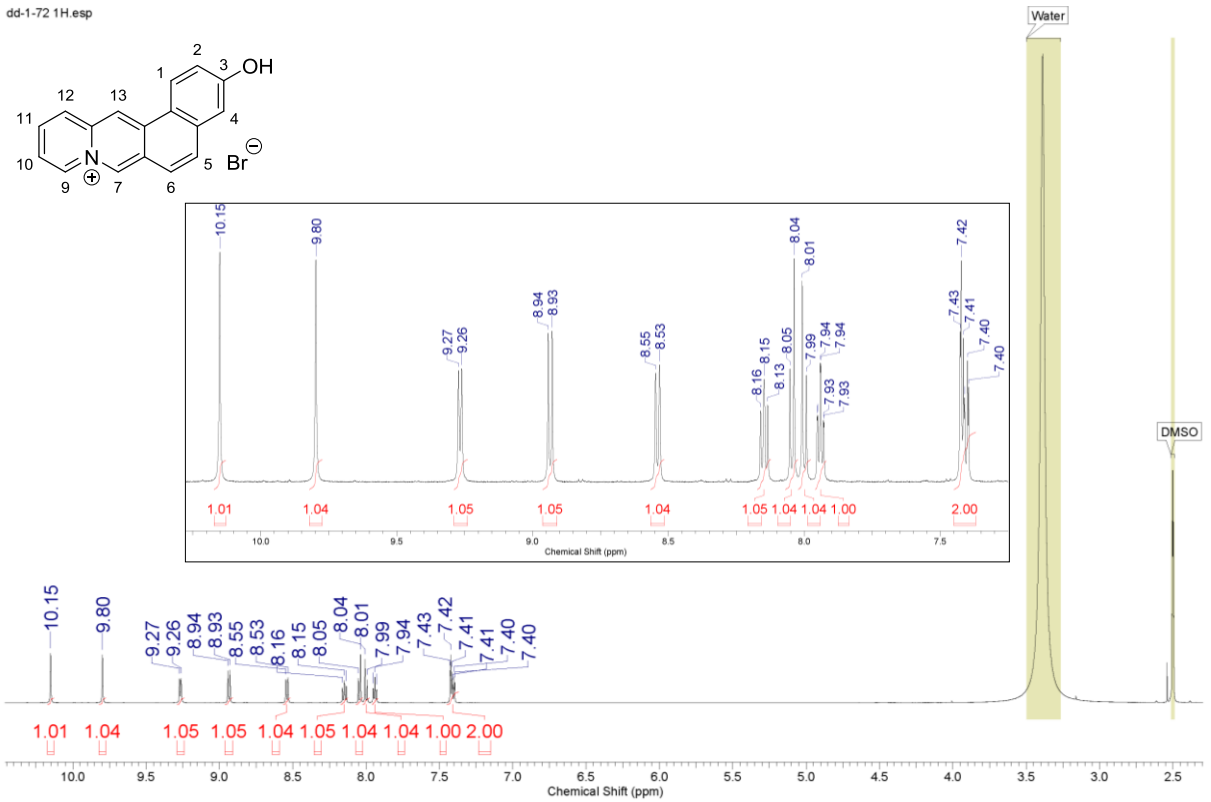

Figure S8: ^{1}H NMR spectrum of 3-hydroxynaphtho[1,2-*b*]quinolizinium bromide (**2**).

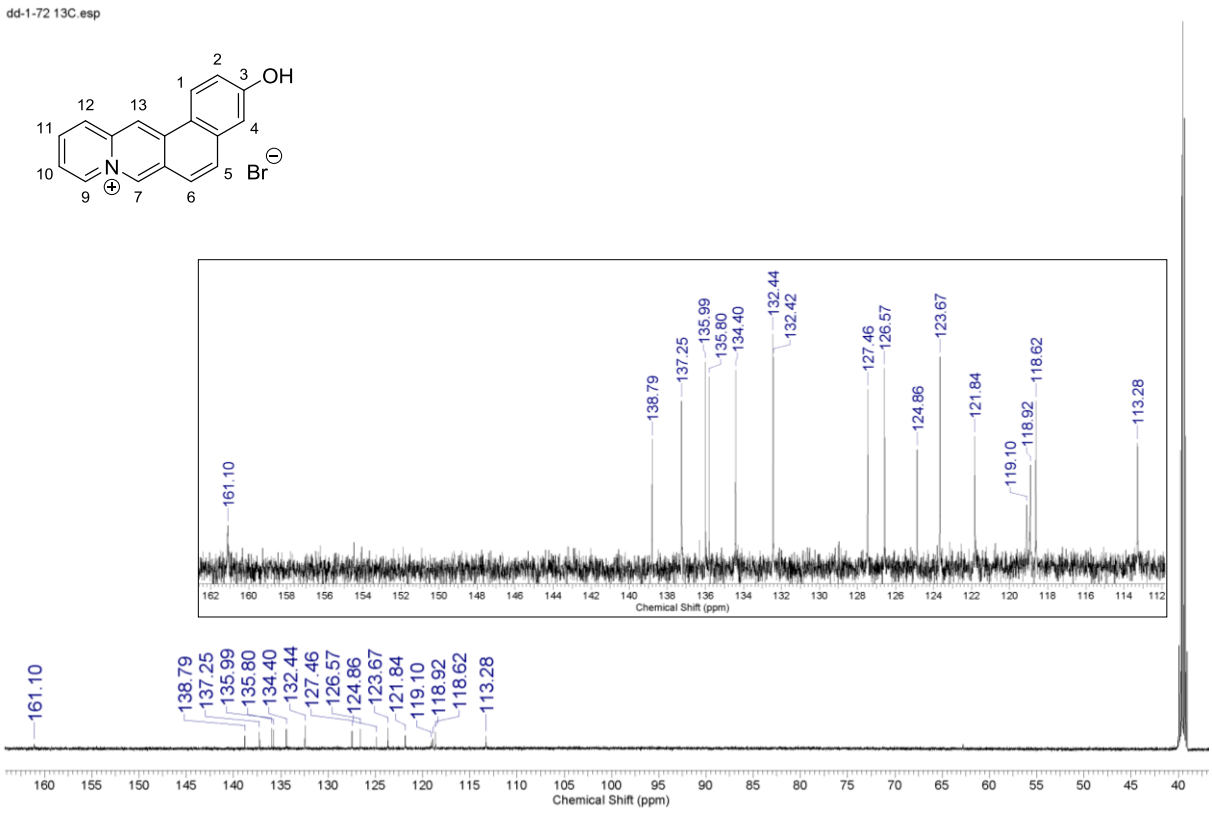

Figure S9: ^{13}C NMR spectrum of 3-hydroxynaphtho[1,2-*b*]quinolizinium bromide (**2**).