

## Electronic Supplementary Information

### **Modulation of $pK_a$ by cyclodextrins; subtle structural changes induce spectacularly different behaviors**

*Paweł M. Nowak<sup>a</sup>, Michał Woźniakiewicz<sup>a\*</sup>, Mariusz P. Mitoraj<sup>b</sup>, Magdalena Garnysz<sup>a</sup>, Paweł Kościelniak<sup>a</sup>*

- a. Department of Analytical Chemistry, Faculty of Chemistry, Jagiellonian University, R. Ingardena 3,  
30-060 Krakow, Poland.
  
- b. Department of Theoretical Chemistry, Faculty of Chemistry, Jagiellonian University, R. Ingardena 3,  
30-060 Krakow, Poland

Table S-1. Composition and predicted pH of all BGEs (background electrolytes) prepared for experiments, calculated for 50 mL total volume and 100 mM ionic strength.

<b>pH</b>	<b>Buffer composition [mL]</b>	
Phosphate buffer I	H <sub>3</sub> PO <sub>4</sub> (100 mM)	NaH <sub>2</sub> PO <sub>4</sub> (100 mM)
2.50	18.52	4.80
3.50	1.83	4.98
Acetic buffer	CH <sub>3</sub> COOH (500 mM)	CH <sub>3</sub> COONa (500 mM)
4.50	14.16	10.00
5.50	1.42	10.00
Phosphate buffer II	NaH <sub>2</sub> PO <sub>4</sub> (100 mM)	Na <sub>2</sub> HPO <sub>4</sub> (100 mM)
6.00	3.59	4.70
7.00	1.01	13.29
8.00	0.12	16.25
Borate buffer	Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> ·10H <sub>2</sub> O (50 mM)	NaOH (1 M)
9.20	48.42	0.16

Above data were obtained from the PHoEBuS 1.3 software by Analis (Namur, Belgium).