

SUPPORTING MATERIAL FOR: INCREASING THE SENSITIVITY OF MICROFLUIDICS BASED IMMUNOASSAYS USING ISOTACHOPHORESIS

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SIMULATION OF ITP

The electromigration of species in the microchannel was modeled using the open source simulation tool Spresso v.2.2 [1]. In the simulation a 3.5 mm long channel with a 50 μm wide and 20 μm deep D-shaped profile was assumed, with sample injection at a position 7.5 mm from the TE reservoir. A current of 10 μA was applied along the channel. The LE and TE consisted of 0.05 mM hydrochloric acid and E-aminocaproic acid, respectively, with 0.1 M ethanolamin as background electrolyte. In order to assure numerical stability, the initial sample concentration was chosen wider than the 50 μm wide injection zone used in the experiment. The reported initial sample concentrations correspond to the experimentally relevant 50 μm wide injection zone and care was taken to let the sample concentration evolve out of the injection zone for the reported shapes during ITP. The valence, mobility and pKa values of the different species used in the simulation are shown in table 1. The values for BSA are chosen such that the mobility and diffusivity roughly match the experimental values reported in [2] in the relevant pH range. Since the purpose of the simulation is to get approximate information on the sample peak shape, in particular about whether the ITP is expected to operate in peak or plateau mode, this rough approximation is sufficient.

Species	z	Mobility ($10^{-9}\text{m}^2\text{s/V}$)	pKa
Hydrochloric acid	-1	79.1	-2.0
E-Aminocaproic Acid	-1	28.8	10.75
	1	28.8	4.373
Ethanolamin	1	44.3	9.498
BSA	-1	3.	4.7
	-2	6.	5
	-3	9.	6
	-4	12.	7
	-5	15.	8
	-6	18.	9

Table 1: Valence, mobility and pKa values of species used in the simulation.

REFERENCES

- [1] M. Bercovici, S.K. Lele, and J.G. Santiago, *J. Chromatogr. A*, 2009, **1216**, 1008-1018.
[2] B.R. Ware, and W. H. Flygare, *Chem. Phys. Lett.*, 1971, **12**, 1, 81-85.