Electronic Supplementary Material for PCCP

Supplementary information

Electrochemical multi-tagging of cysteinyl peptides during microspray mass spectrometry: numerical simulation of consecutive reactions in a microchannel

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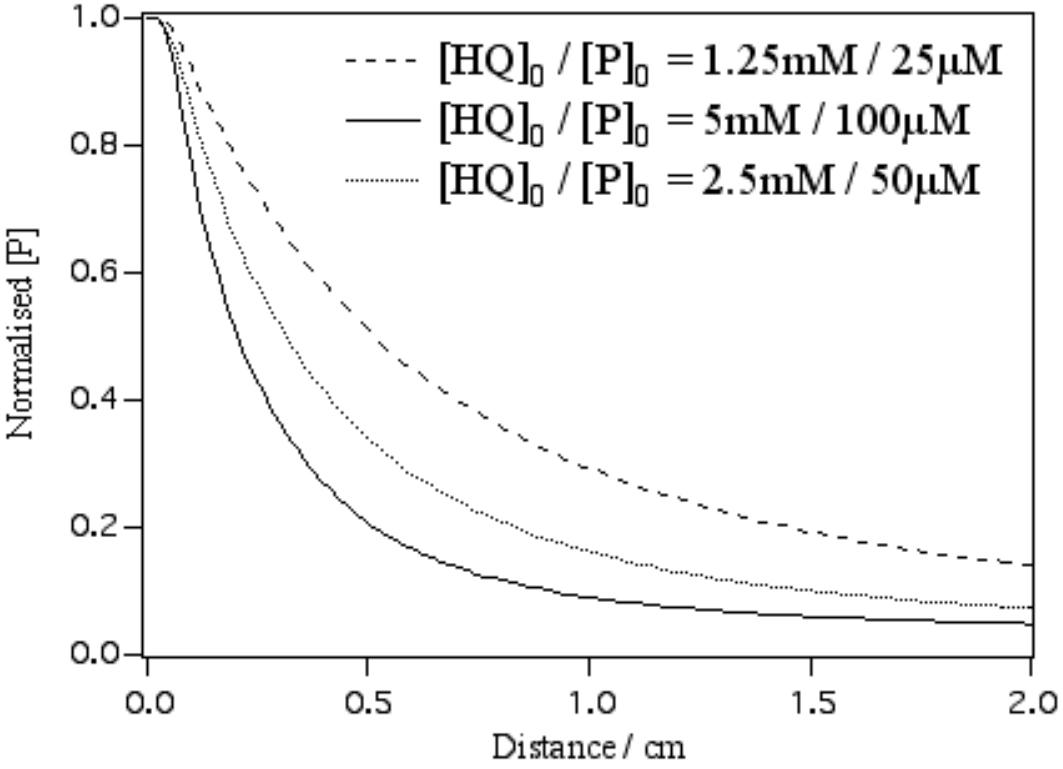

Figure S1. Kinetics of the tagging (evolution of [P] / $[P]_0$) for several initial concentrations of HQ and P in the case of a three-cysteine-containing biomolecule. The ratio $[HQ]_0$ / $[P]_0$ is kept constant.

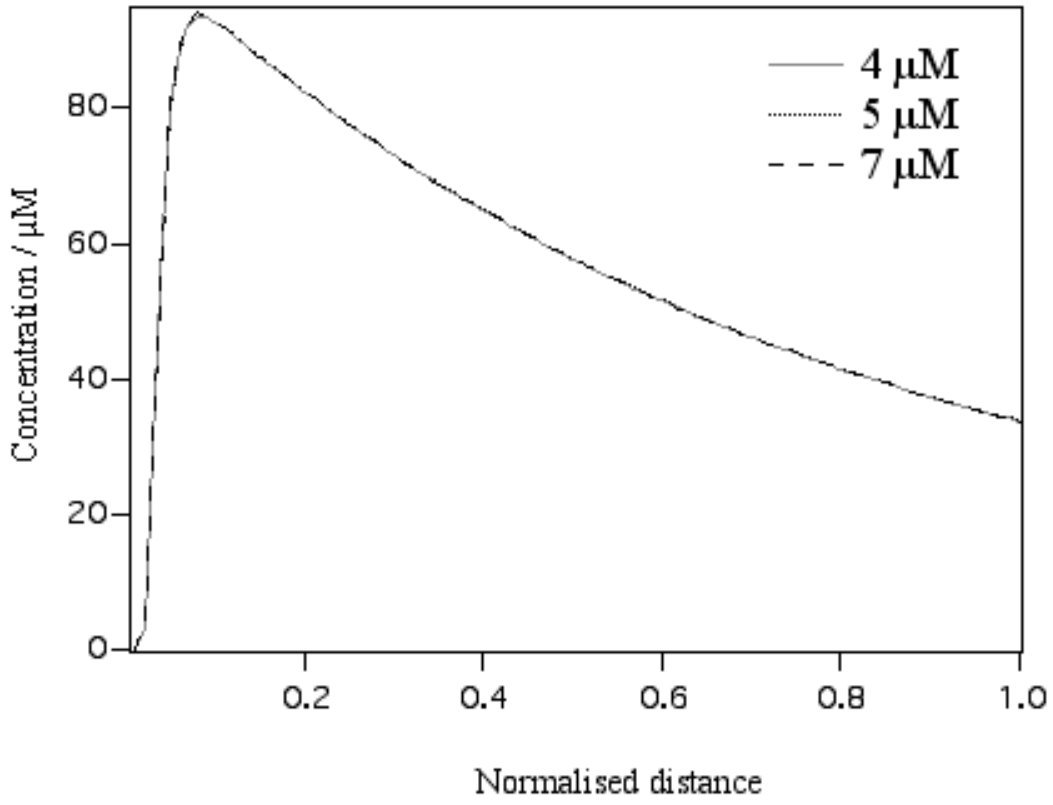

Figure S2. Meshing validation by comparison of BQ concentration along the channel with main mesh size of 4 μm, 5 μm and 7 μm.

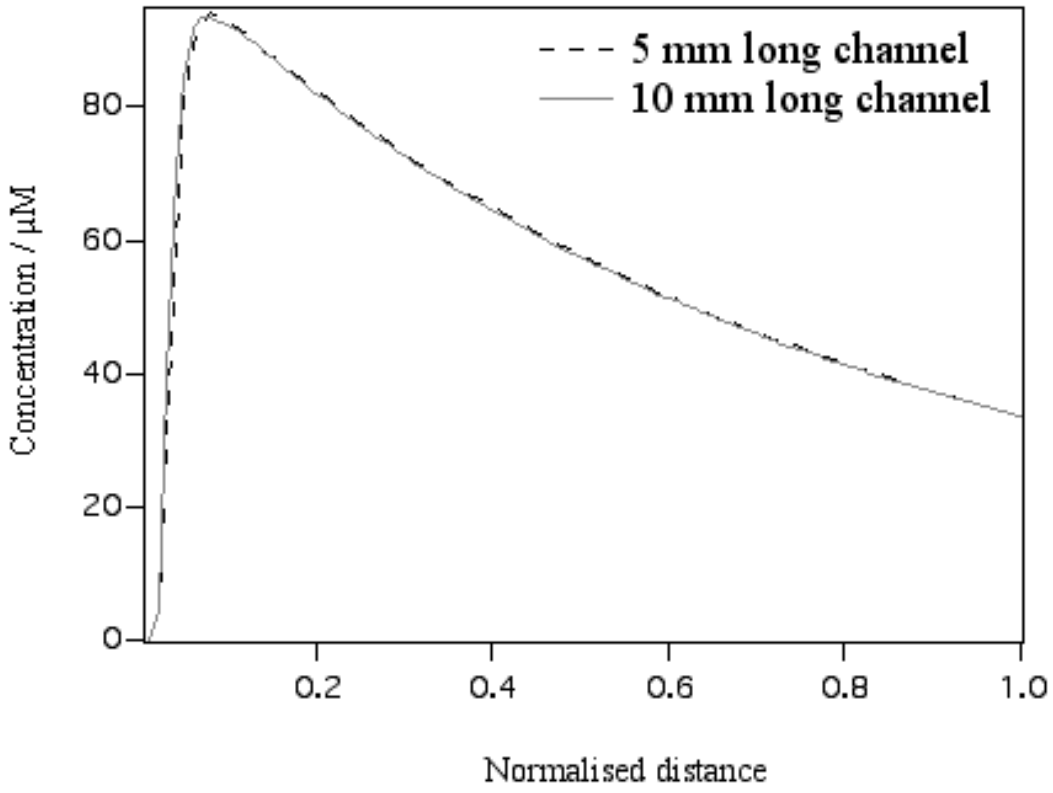

Figure S3. Scaling validation by comparison of BQ concentrations along the channel for a scaling by 2 (channel length of 10 mm) and by 4 (channel length of 5 mm). The flow rate of the fluid was adapted to conserve the flux of species.

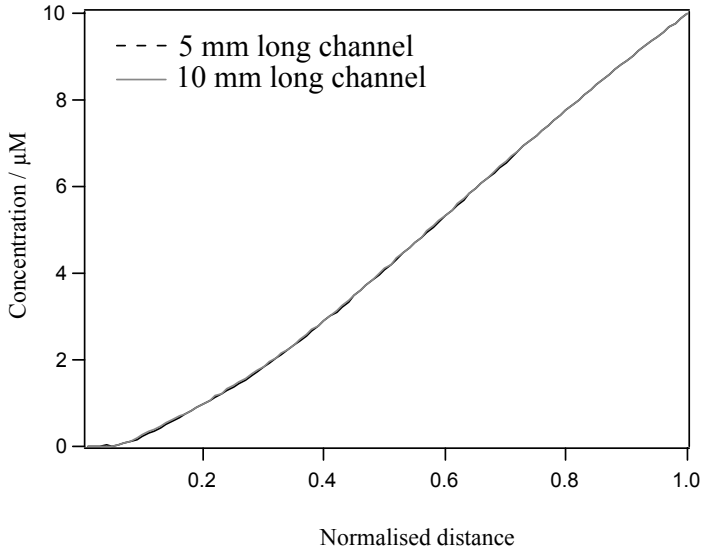

Figure S4. Scaling validation by comparison of PQ_3 concentrations (three-cysteine-containing target simulation) along the channel for a scaling by 2 (channel length of 10 mm) and by 4 (channel length of 5 mm). The flow rate of the fluid was adapted to conserve the flux of species.

HQ	BQ	P	PQ_1	PQ_2	PQ_3	PQ_4	PQ_5
$D_Q\nabla\alpha\nabla\beta$ $+\alpha\boldsymbol{v}\nabla\beta$ $+\alpha k_{ox}\beta$	$-\alpha k_{red}\beta$						
$-\alpha k_{ox}\beta$	$D_Q\nabla\alpha\nabla\beta$ $+\alpha\boldsymbol{v}\nabla\beta$ $+\alpha k_{red}\beta$ $+\alpha k_1 c_P\beta$ $+\alpha k_2 c_{PQ1}\beta$ $+\alpha k_3 c_{PQ2}\beta$ $+\alpha k_4 c_{PQ3}\beta$ $+\alpha k_5 c_{PQ4}\beta$						
		$D_P\nabla\alpha\nabla\beta$ $+\alpha\boldsymbol{v}\nabla\beta$ $+\alpha k_1 c_{BQ}\beta$					
		$-\alpha k_1 c_{BQ}\beta$	$D_P\nabla\alpha\nabla\beta$ $+\alpha\boldsymbol{v}\nabla\beta$ $+\alpha k_2 c_{BQ}\beta$				
			$-\alpha k_2 c_{BQ}\beta$	$D_P\nabla\alpha\nabla\beta$ $+\alpha\boldsymbol{v}\nabla\beta$ $+\alpha k_3 c_{BQ}\beta$			
				$-\alpha k_3 c_{BQ}\beta$	$D_P\nabla\alpha\nabla\beta$ $+\alpha\boldsymbol{v}\nabla\beta$ $+\alpha k_4 c_{BQ}\beta$		
					$-\alpha k_4 c_{BQ}\beta$	$D_P\nabla\alpha\nabla\beta$ $+\alpha\boldsymbol{v}\nabla\beta$ $+\alpha k_5 c_{BQ}\beta$	
						$-\alpha k_5 c_{BQ}\beta$	$D_P\nabla\alpha\nabla\beta$ $+\alpha\boldsymbol{v}\nabla\beta$

Figure S5. The M_{ij} steady state matrix is described. All the gradients are written in a nabla form ∇. The function β is the interpolation function of the unknown. The position in the matrix of the reaction terms is chosen to maximize the weight of the diagonal.