Table S3. Statistical parameters characterizing bimodal computer-simulated pH distributions.

	A	B	C	D	E	F
weighted mean, $\overline{pH_e}$	6.85	6.92	7.03	7.10	7.15	7.20
weighted median, $\widetilde{pH}_e$	6.85	7.01	7.11	7.16	7.18	7.20
mode, pH_{e1}	7.20	7.20	7.20	7.20	7.20	7.20
mode, pH_{e2}	6.50	6.50	6.50	6.50	6.55	n.d.
intensity ratio pH_{e2}/pH_{e1}	1.00	0.67	0.33	0.17	0.08	0.0001
area ratio pH_{e2}/pH_{e1}						
- integrated	1.00	0.64	0.31	0.15	0.06	n.d.
- rel. error [%]	0	-4.5	-6.1	-11.8	-25	n.d.
- integration limit [pH]	6.85	6.80	6.75	6.70	6.60	n.d.
skewness, G1	0.00	-0.26	-0.67	-0.95	-1.01	0.00
kurtosis, G2	-1.14	-1.02	-0.33	0.78	1.75	0.01
entropy, H	4.90	4.87	4.73	4.54	4.37	4.05

Data are based on the simulated Gaussian pH distributions presented in Fig. S5. Curves were numerically generated based on intervals of 0.05 pH units, such that pH modes coincided with nominal pH values of 7.20 (pH_{e1}) and 6.50 (pH_{e2}). The modes, pH_{e1} and pH_{e2}, were added with pH_{e2}/pH_{e1} proportions (intensity ratios) decreasing from A to F (see also Figure S4 panels A to F). For equal pH_{e1} and pH_{e2} contributions (A), the pH_e distribution was broad (low kurtosis and high entropy) and perfectly symmetric (skewness = 0); $\overline{pH_e}$ and $\widetilde{pH}_e$ had identical values, and the ratio of the pH_{e2} area *vs.* the pH_{e1} area obtained by integration had the theoretical value of 1.00. With decreasing pH_{e2} contribution (B to F), the distribution curve became more pointed (increased kurtosis), less even (decreased entropy), and asymmetric (negative skewness); moreover, $\overline{pH_e}$ and $\widetilde{pH}_e$ diverged ($\overline{pH_e} < \widetilde{pH}_e$), and the area ratios pH_{e2}/pH_{e1} became smaller than the corresponding theoretical values (Figure S4 panel G).
The apparent position of the pH_{e2} mode tended to be shifted to slightly increased values for low intensity ratios (column E). However, for extremely small pH_{e2} contributions (column F; Fig. S4 F), the pH profile became symmetric about pH_{e1} (vanishing G1), $\overline{pH_e} = \widetilde{pH}_e = pH_{e1}$, and G2 vanished as the overall pH distribution approached a single Gaussian distribution. Consequently, also the evenness of the pH curve approached that of a single Gaussian (H = 4.05) as the pH_{e2} contribution became virtually undetectable.