Supporting Information

Table SI.1 Ion selective electrode (ISE) hardware

Analyte	Membrane	Manufacturer / Model	Published range limit [M]
Ca^{2+}	Solid-state PVC polymer matrix	ELIT 8041	$5{\cdot}10^{-7}$ (0.02 ppm)
K^{+}	Solid-state PVC polymer matrix	ELIT 8031	$1{\cdot}10^{-5}$ (0.4 ppm)
Na^{+}	Solid-state PVC polymer matrix	ELIT 8230	$2{\cdot}10^{-6}$ (0.05 ppm)
NH_4^{+}	Solid-state PVC polymer matrix	ELIT 8051	$2{\cdot}10^{-6}$ (0.03 ppm)
Cl^{-}	Solid-state poly-crystalline	ELIT 8261	$3{\cdot}10^{-5}$ (1 ppm)
NO_3^{-}	Solid-state PVC polymer matrix	ELIT 8021	$5{\cdot}10^{-6}$ (0.3 ppm)
Cl^{-}	Solid-state (unspecified)	Hanna Instruments 4007	$5{\cdot}10^{-5}$ (1.8 ppm)
Hardness	Plastic (unspecified)	Thermo Sci. 9332BNWP	$6{\cdot}10^{-6}$
pH	Glass	Thermo Sci. 9101BN	pH 0 - 14
Na^{+}	Glass	Ross 8411BN	$1{\cdot}10^{-6}$ (0.02 ppm)
Reference	double junction CH_3COOLi	ELIT 003N	

Table SI.2 Most informative calibration curve for estimation of ion concentration directly using a single ISE with a log-linear calibration (log-linear range listed). Detection Limit (LOD) is listed as the concentration below which response cannot be differentiated from the noise baseline (3σ); approximate LOD is listed for electrodes for which lowest measured standard did not yet appear to have reached the noise baseline.

Ion	ISE	slope [mV/decade]	intercept [mV]	Range limit [M]	R^2	RMSE	LOD [M]
Na^{+}	**ELIT Na^{+}**	52.7	500.6	$2{\cdot}10^{-6}$	0.999	3.31	$<5{\cdot}10^{-7}$
K^{+}	**ELIT K^{+}**	55.5	548	$2.5{\cdot}10^{-7}$	0.998	4.53	$<2.5{\cdot}10^{-7}$
Ca^{2+}	**ELIT Ca^{2+}**	33.9	388.9	$2.5{\cdot}10^{-6}$	0.981	7.95	$1.3{\cdot}10^{-6}$
Mg^{2+}	**Hardness**	23.6	74.1	$2.5{\cdot}10^{-5}$	>0.999	0.6	$5{\cdot}10^{-6}$
NH_4^{+}	**ELIT NH_4^{+}**	57	582.7	$1{\cdot}10^{-6}$	0.998	4.4	$<1{\cdot}10^{-6}$
Cl^{-}	**ELIT Cl^{-}**	-53.8	-0.014	$2{\cdot}10^{-5}$	0.998	2.85	$3{\cdot}10^{-6}$
NO_3^{-}	**ELIT NO_3^{-}**	-56.2	192.6	$1{\cdot}10^{-5}$	0.999	2.85	$3{\cdot}10^{-6}$

Table SI.3 Parameterization for best ANN (selected using NRMSE metric).

Hidden Layers	[6,18,15]
Output Layers	3 (ion concentrations, EC, CB)
Hidden layer transfer function	tansig
Output layer transfer function	purelin
Training goal	10^{-6}
Max. # of epochs	10,000
μ	0.001
μ_{dec}	0.1
μ_{inc}	10
Training fraction	0.7
Validation fraction	0.15
Testing fraction	0.15

Artificial Neural Network Method Summary An ANN is a non-linear function estimator comprised of a number of interconnected neurons, wherein the number of neurons and strength of interconnections are both critical to the model. *Input* neuron signals are processed successively by a number of *hidden* neuron layers, each of which can have any number of neurons, before activating signals at the *output* neurons; typically each neuron receives weighted input signals from all neurons in the preceding layer (most commonly mathematically combined using the dot product) and provides an output signal fed to all neurons in the subsequent layer (produced by passing the received signal through a *transfer function*, usually a highly non-linear function such as a hyperbolic tangent sigmoid). Initial neuron interconnections and strengths are specified by the system designer, however weights of interconnections are adapted during *training* (successive presentation of matched input and output data pairs) and can drop to zero (*prune* unnecessary interconnections). Backpropagation techniques (see Fig. SI.1 are used to update system parameters based on error between the output neuron signals and the target (desired output) signals provided to the system at each iteration (each presentation of an input/output data pair). The designer sets the number of hidden layers, number of nodes per layer, transfer functions, learning rates, and training algorithm.

Network inputs and outputs are typically normalized before training, to equalize the effect of each channel on the output RMSE calculation, e.g., to values between ± 1. The broad methodology followed in neural network training is shown in Fig. SI.1. The data used as inputs and targets during training are termed the *training set*, while independent pairs of input/target data are typically reserved for *validating* and/or *testing* the network 'goodness' (metric may be MAE, MSE, RMAE, or RMSE) in addition to preventing overtaining (the case in which network prediction is tuned well for the training set but produces poor results on other samples).

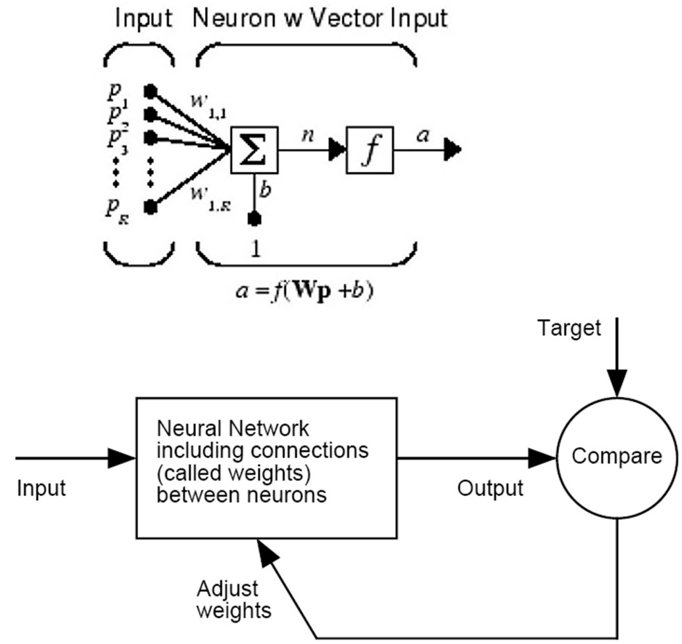

Fig. SI.1 ANN prototypical neuron and training methodology.