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Perspectives on: Ion selectivity
Design principles for K^+ selectivity in membrane transport

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Please note that Yu et al. (2010. *J. Amer. Chem. Soc.* 132:10847–10856) cited the wrong LJ parameter set used for Na^+ and K^+ ions (Andersen, O.S., and B. Roux, personal communication). In their study, Yu et al. (2010) did not use the parameter set from Beglov and Roux (1994. *J. Chem. Phys.* 100:9050–9063), but instead the parameter set from Noskov and Roux (2008. *J. Mol. Biol.* 377:804–818). These two parameter sets yield different $K^+ \rightarrow Na^+$ hydration free energy differences. While the parameters from Beglov and Roux (1994) yield a value of −20.7 kcal/mol, the parameters from Noskov and Roux (2008) yield a value of −18.6 kcal/mol. This consequently modifies two entries in Table I (marked by asterisks below), but has no impact on the published conclusions.

TABLE I

K^+/Na^+ selectivity by experiment and calculation

Method	Solvent	ΔΔG (kcal/mol)	Selective for
Experiment	Formamide[a]	−0.9	Na^+
	Formamide[b,c]	−0.7	Na^+
	NMA[b,d]	−1.1	Na^+
Pairwise Additive	Formamide[c] (CHARMM27)	0.9	K^+
	Formamide[c] (OPLS-AA)	1.3	K^+
	NMA[c] (CHARMM22/NBFIX)	1.6	K^+
	NMA[d,g] (CHARMM27)	0.7*	K^+
	NMA[d,g] (CHARMM27/NBFIX)	2.6*	K^+
Polarizable	Formamide[c] (AMOEBA)	−1.3	Na^+
	Formamide[f] (QM/MM)	−2.2	Na^+
	NMA[d] (Drude)	−0.3	Na^+

K^+/Na^+ selectivity of bulk liquid formamide and NMA as determined by experimental work, pairwise-additive (nonpolarizable) force field calculations, polarizable force field (AMOEBA and Drude) calculations, and QM/MM (hybrid quantum mechanical and molecular mechanical) calculations. Note that the pairwise-additive force field calculations display positive (K^+) selectivity, whereas all other determinations display negative (Na^+) selectivity.

[a]Marcus, 1983.
[b]Cox and Parker, 1973, and Schmid et al., 2000.
[c]Grossfield et al., 2003.
[d]Yu et al., 2010a.
[e]Noskov et al., 2004.
[f]Varma and Rempe, 2008.
[g]Noskov and Roux, 2008.