

Corrections

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2011. The role of bulk protein in local models of ion-binding to proteins: Comparative study of KcsA, its semisynthetic analog with a locked-in binding site, and valinomycin. *Biophys. J.* 100:1542–1549.

In Tables 1 and 3, we incorrectly noted three energy values. We rectify those errors here. The changes are small and do not affect the conclusions in the article.

In Table 1 for wild-type KcsA in column A₃, $\Delta\langle\epsilon_{\text{local}}\rangle$ is -21.0 not -19.6 .

In Table 3 for wild-type KcsA, the ion site interactions, $\Delta\langle\epsilon_{\text{local}}\rangle$ is -21.0 not -19.6 .

In Table 3 for wild-type KcsA, the ion-medium interactions, $\Delta\langle\epsilon_{\text{m}}\rangle$ is 2.2 not 0.8 .

In Table 3 for wild-type KcsA, the local entropy change, $T\Delta S_{\text{local}}^{\text{ex}}$ is 2.1 not 3.5 .

We reproduce Tables 1 and 3 here for completeness. The updated values are noted in bold.

TABLE 1 Free energy and binding energy for KcsA, KcsA-G77A_D, and valinomycin according to three different methods of assessing ion-protein interactions (see Methods)

	A ₁	A ₂	A ₃
KcsA			
$\Delta\mu^{\text{ex}}(\text{S})/\Delta W_{\text{local}}$	-14.7	-15.7	-15.8
$\Delta\langle\epsilon_{\text{local}}\rangle$	-20.9	-18.8	-21.0
KcsA-G77A_D			
$\Delta\mu^{\text{ex}}(\text{S})/\Delta W_{\text{local}}$	-9.0	-10.0	-9.9
$\Delta\langle\epsilon_{\text{local}}\rangle$	-28.3	-19.3	0.8
Valinomycin			
$\Delta\mu^{\text{ex}}(\text{S})/\Delta W_{\text{local}}$	-11.3		-11.0
$\Delta\langle\epsilon_{\text{local}}\rangle$	-17.7		-9.4

ΔW_{local} is insensitive to these choices and is sufficiently close to the actual free energy change, $\Delta\mu^{\text{ex}}(\text{S})$. The local model adequately captures binding energetics in KcsA but not in KcsA-G77A_D and valinomycin. For the latter two systems, Na⁺ is stabilized by interactions with medium outside the binding site. Statistical uncertainties in energy values are ~ 0.8 kcal/mol.

TABLE 3 Energetic decomposition for KcsA and KcsA-G77A_D

	KcsA	KcsA-G77A _D	
$\Delta\mu^{\text{ex}}(\text{S})$	-15.7	-10.0	
ΔW_{local}	-15.8	-9.9	
$T\Delta S^{\text{ex}}$	1.3	-1.1	
$T\Delta S_{\text{local}}^{\text{ex}}$	2.1	4.7	
Ion-site	$\Delta\langle\epsilon_{\text{local}}\rangle$	-21.0	0.8
Ion-medium	$\Delta\langle\epsilon_{\text{m}}\rangle$	2.2	-20.1
Site-site	$\Delta\langle U_{\text{S}}\rangle$	7.3	-6.0
Site-medium	$\Delta\langle U_{\text{S-M}}\rangle$	-2.9	14.5
Medium-medium	$\Delta\langle U_{\text{M}}\rangle$	0.0	-0.3

Eight carbonyl ligands comprise the local site. We consider the water molecules in the S₁ and S₃ sites adjoining the S₂ site as the medium. Similar to valinomycin, the change in ion-medium interactions is inversely related to the change in site-medium interactions. All values are in kcal/mol.

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Author L. B. Dyksterhuis' middle initial is incorrect in the published article and is corrected here.

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