

SUPPLEMENTAL MATERIAL

JGP

Bailey et al., <http://www.jgp.org/cgi/content/full/jgp.201010430/DC1>

Table S1 follows and shows results from the sensitivity analysis.

TABLE S1

Sensitivity Analysis KCa3.1: linear dependence on Ca^{2+} concentration, $k=A\cdot[\text{Ca}]$. Data set #1

Kinetic Transition	Rate Constant	Change in Error +10% rate constant	Change in Error -10% rate constant
<hr/>			
12	$7\ \mu\text{M}^{-1}\ \text{s}^{-1}$	14%	17%
21	$36\ \text{s}^{-1}$	10%	12%
23	$1200\ \mu\text{M}^{-1}\ \text{s}^{-1}$	13%	16%
32	$230\ \text{s}^{-1}$	13%	16%
34	*	*	*
43	*	*	*
35	$35\ \text{s}^{-1}$	51%	58%
53	$16\ \text{s}^{-1}$	50%	61%
46	*	*	*
64	*	*	*

total error = 31

Sensitivity Analysis KCa3.1: non-linear dependence on Ca^{2+} concentration, $k=A\cdot[\text{Ca}]/(B+[\text{Ca}])$. Data set #1

Kinetic Transition	Rate Constant	Change in Error	Change in Error
		+10% rate constant	-10% rate constant
12	$30\ \mu\text{M}^{-1}\ \text{s}^{-1}$	10%	5%
21	$26\ \text{s}^{-1}$	4%	7%
23	$2700\ \mu\text{M}^{-1}\ \text{s}^{-1}$	10%	9%
32	$230\ \text{s}^{-1}$	8%	12%
34	*	*	*
43	*	*	*
35	$27\ \text{s}^{-1}$	37%	35%
53	$15\ \text{s}^{-1}$	30%	45%
46	*	*	*
64	*	*	*
			total error = 38

Sensitivity Analysis KCa3.1: linear-dependence on Ca^{2+} concentration, $k=A\cdot[\text{Ca}]$. Data set #2 (paired)

Kinetic Transition	Rate Constant	Change in Error +10% rate constant	Change in Error -10% rate constant
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12	$5\ \mu\text{M}^{-1}\ \text{s}^{-1}$	8%	10%
21	$21\ \text{s}^{-1}$	4%	6%
23	$1740\ \mu\text{M}^{-1}\ \text{s}^{-1}$	6%	8%
32	$280\ \text{s}^{-1}$	7%	8%
34	*	*	*
43	*	*	*
35	$32\ \text{s}^{-1}$	37%	44%
53	$21\ \text{s}^{-1}$	38%	43%
46	*	*	*
64	*	*	*

total error = 38

Sensitivity Analysis KCa3.1: non-linear dependence on Ca^{2+} concentration, $k=A\cdot[\text{Ca}]/(B+[\text{Ca}])$. Data set #2
(paired)

Kinetic Transition	Rate Constant	Change in Error +10% rate constant	Change in Error -10% rate constant
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12	$24\ \mu\text{M}^{-1}\ \text{s}^{-1}$	8%	11%
21	$42\ \text{s}^{-1}$	6%	6%
23	$8150\ \mu\text{M}^{-1}\ \text{s}^{-1}$	6%	9%
32	$150\ \text{s}^{-1}$	7%	7%
34	*	*	*
43	*	*	*
35	$39\ \text{s}^{-1}$	34%	42%
53	$24\ \text{s}^{-1}$	36%	40%
46	*	*	*
64	*	*	*
			total error = 38
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Sensitivity Analysis KCa3.1+PCMBs: linear dependence on Ca^{2+} concentration, $k=A\cdot[\text{Ca}]$. Data set #2

(paired)

Kinetic Transition	Rate Constant	Change in Error +10% rate constant	Change in Error -10% rate constant
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12	$5\ \mu\text{M}^{-1}\ \text{s}^{-1}$	1%	2%
21	$23\ \text{s}^{-1}$	1%	1%
23	$550\ \mu\text{M}^{-1}\ \text{s}^{-1}$	1%	2%
32	$660\ \text{s}^{-1}$	1%	1%
34	*	*	*
43	*	*	*
35	$290\ \text{s}^{-1}$	1%	2%
53	$4\ \text{s}^{-1}$	2%	2%
46	*	*	*
64	*	*	*

total error = 64

Sensitivity Analysis KCa3.1+PCMBs: non-linear dependence on Ca^{2+} concentration, $k=A\cdot[\text{Ca}]/(B+[\text{Ca}])$.

Data set #2 (paired)

Kinetic Transition	Rate Constant	Change in Error +10% rate constant	Change in Error -10% rate constant
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12	$10\ \mu\text{M}^{-1}\ \text{s}^{-1}$	4%	3%
21	$76\ \text{s}^{-1}$	3%	3%
23	$2900\ \mu\text{M}^{-1}\ \text{s}^{-1}$	3%	4%
32	$2980\ \text{s}^{-1}$	3%	4%
34	*	*	*
43	*	*	*
35	$290\ \text{s}^{-1}$	3%	4%
53	$3\ \text{s}^{-1}$	5%	4%
46	*	*	*
64	*	*	*

total error = 45

Sensitivity Analysis KCa3.1+PCMBS constrained: non-linear dependence on Ca⁺ concentration,

$$k=A\cdot[Ca]/(B+[Ca]).$$

Kinetic Transition	Rate Constant	Change in Error	
		+10% rate constant	-10% rate constant
12	*27 $\mu\text{M}^{-1} \text{s}^{-1}$	2%	2%
21	*34 s^{-1}	1%	1%
23	*5425 $\mu\text{M}^{-1} \text{s}^{-1}$	1%	2%
32	*190 s^{-1}	2%	2%
34	*	*	*
43	*	*	*
35	*34 s^{-1}	3%	5%
53	3 s^{-1}	5%	4%
46	*	*	*
64	*	*	*
total error = 43			

*Transitions 12, 21, 23, 32, 35 are fixed to the average value from KCa3.1 (without PCMBS) data sets #1 and #2.

Sensitivity Analysis KCa3.1 L281W: non-linear dependence on Ca^+ concentration, $k=A\cdot[\text{Ca}]/(B+[\text{Ca}])$.

Kinetic Transition	Rate Constant	Change in Error	Change in Error
		+10% rate constant	-10% rate constant
12	$11\ \mu\text{M}^{-1}\ \text{s}^{-1}$	0.3%	0.3%
21	$76\ \text{s}^{-1}$	0.2%	0.2%
23	$12380\ \mu\text{M}^{-1}\ \text{s}^{-1}$	0.2%	0.2%
32	$192\ \text{s}^{-1}$	0.2%	0.2%
34	*	*	*
43	*	*	*
35	$53\ \text{s}^{-1}$	2%	3%
53	$5\ \text{s}^{-1}$	3%	3%
46	*	*	*
64	*	*	*
total error = 8			

Sensitivity Analysis KCa3.1 L281W constrained: non-linear dependence on Ca⁺ concentration,

$$k=A\cdot[Ca]/(B+[Ca]).$$

Kinetic Transition	Rate Constant	Change in Error	
		+10% rate constant	-10% rate constant
12	*27 $\mu\text{M}^{-1} \text{s}^{-1}$	0.2%	0.2%
21	*34 s^{-1}	0.2%	0.1%
23	*5425 $\mu\text{M}^{-1} \text{s}^{-1}$	0.2%	0.3%
32	*190 s^{-1}	0.0%	0.2%
34	*	*	*
43	*	*	*
35	*34 s^{-1}	2%	2%
53	4 s^{-1}	1%	3%
46	*	*	*
64	*	*	*
total error = 13			

*Transitions 12, 21, 23, 32, 35 are fixed to the average value from KCa3.1 (without PCMBs) data sets #1 and #2.

Shaker	#458	V G S L C A I A G V L T I A L P V P V I V	#478
KcsA	#91	V A V V V M V A G I T S F G L V T A A L A	#111
KCa3.1	#266	V C L C T G V M G V C C T A L L V A V V A	#286
		<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="border: 1px solid black; padding: 2px;">275</div> <div style="border: 1px solid black; padding: 2px;">278</div> <div style="border: 1px solid black; padding: 2px;">282</div> </div> <div style="border: 1px solid black; height: 20px; width: 50%; margin: 5px auto; text-align: center;">S6</div>	

Sequence alignment between KCa3.1, Shaker, and KcsA illustrating a correspondence between residues Val²⁷⁵ and Thr²⁷⁸ to the known pore lining residues Ile¹⁰⁰ and Phe¹⁰³ in KcsA, and residues Thr²⁷⁸ and Val²⁸² to the known pore lining residues Ile⁴⁰² and Val⁴⁰⁶ in Shaker.