Supporting Information for: The Information Content of Voltage-Dependent Conductance Histograms

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Herein we list the MolStat (version 1.1)[1] input files used to generate each of the histograms in Figures 3, 4, 5, and 7 of the main text. Figure 6 uses the same data as Figure 4. Note that running these files will not generate the *exact* data as that used in the figures since MolStat relies on random number generation and the seeds will likely be different. However, each histogram is constructed from one million conductance "measurements," which should be sufficient for the central limit theorem to apply. Finally, note also that MolStat considers the voltage V to be a random variable. In all of these calculations, we specify a uniform distribution between -2 V and 2 V. To mimic the experimental procedure,[2] each vertical slice of the histogram was rescaled to have the same number of counts. In essence, this normalizes each vertical slice.

Figure 3(b)

```
SymmetricOneSite
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
gamma normal 0.5 0.05
```

Figure 3(c)

```
SymmetricOneSite
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
gamma normal 0.5 0.05
```

Figure 3(d)

```
SymmetricOneSite
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.06
epsilon normal -3. 0.05
gamma normal 0.5 0.05
```

Figure 3(e)

```
SymmetricOneSite
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.06
epsilon normal -3. 0.05
gamma normal 0.5 0.05
```

Figure 4(b)

```
AsymmetricOneSite
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 0.5 0.05
```

Figure 4(c)

```
AsymmetricOneSite
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
```

```
gammaL normal 0.5 0.05
gammaR normal 0.5 0.05
```

Figure 4(d)

```
AsymmetricOneSite
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 0.7 0.05
```

Figure 4(e)

```
AsymmetricOneSite
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 0.7 0.05
```

Figure 4(f)

```
AsymmetricOneSite
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 1.2 0.05
```

Figure 4(g)

```
AsymmetricOneSite
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 1.2 0.05
```

Figure 5(a)

```
AsymmetricOneSite
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.06
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 0.7 0.05
```

Figure 5(b)

```
AsymmetricOneSite
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.06
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 0.7 0.05
```

Figure 5(c)

```
AsymmetricOneSite
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.06
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 1.2 0.05
```

Figure 5(d)

```
AsymmetricOneSite
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.06
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 1.2 0.05
```

Figure 6(a), Red Line

```
AsymmetricOneSite
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 2. 0.05
```

Figure 6(b), Red Line

```
AsymmetricOneSite
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a constant 0.
epsilon normal -3. 0.05
gammaL normal 0.5 0.05
gammaR normal 2. 0.05
```

Figure 7(a)

```
IndependentTwoChannel
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a1 constant 0.2
epsilon1 normal -3.5 0.3
gamma1 normal 0.08 0.015
a2 constant 0.1
epsilon2 normal -3.8 0.3
gamma2 normal 0.11 0.015
```

Figure 7(b)

```
IndependentTwoChannel
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a1 constant 0.2
epsilon1 normal -3.5 0.3
gamma1 normal 0.08 0.015
a2 constant 0.1
epsilon2 normal -3.8 0.3
gamma2 normal 0.11 0.015
```

Figure 7(c)

```
IndependentTwoChannel
StaticConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a1 constant -0.8
epsilon1 normal -3.5 0.3
gamma1 normal 0.08 0.015
a2 constant 0.5
epsilon2 normal -3.8 0.3
gamma2 normal 0.11 0.015
```

Figure 7(d)

```
IndependentTwoChannel
DifferentialConductance
1000000
100 log 10.
ef constant 0.
V uniform -2. 2.
a1 constant -0.8
epsilon1 normal -3.5 0.3
gamma1 normal 0.08 0.015
a2 constant 0.5
epsilon2 normal -3.8 0.3
gamma2 normal 0.11 0.015
```

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[1] https://bitbucket.org/mgreuter/molstat.

[2] S. Guo, J. Hihath, I. Díez-Pérez, and N. Tao, J. Am. Chem. Soc. **133**, 19189 (2011).