**TABLE 1 Calculated all-atom MD simulation results in DPhPC and DPPC bilayers at 330 K**

| Lipid | Ion | $W_{peak,calc}$ (kcal/mol) | $D_{mem}/D_{Bulk}$ (Å$^2$/ps) | $P_{ion,calc}$ ($\times 10^{-12}$ cm/s) | log$P_{ion,calc}$ (log(cm/s)) | $G_{ion,calc}$ (nS/cm$^2$) |
|---|---|---|---|---|---|---|
| DPhPC | $GuanH^+$ | 24.0 ± 0.5 | 0.011 ± 0.004/0.31 ± 0.03 | 0.020 ± 0.025 | −13.70 ± 0.31 | 0.068 ± 0.085 |
| DPPC | $GuanH^+$ | 24.6 ± 0.4 | 0.017 ± 0.004/0.31 ± 0.03 | 0.011 ± 0.014 | −13.97 ± 0.28 | 0.037 ± 0.049 |
| | $K^+$ | 25.8 ± 0.1 | 0.030 ± 0.012/0.40 ± 0.05 | 0.0023 ± 0.0022 | −14.64 ± 0.21 | 0.0078 ± 0.0076 |
| | $Na^+$ | 25.6 ± 0.2 | 0.017 ± 0.010/0.30 ± 0.04 | 0.0014 ± 0.0026 | −14.85 ± 0.44 | 0.0048 ± 0.0089 |
| | $Cl^-$ | 24.1 ± 0.3 | 0.047 ± 0.012/0.44 ± 0.06 | 0.033 ± 0.024 | −13.49 ± 0.30 | 0.111 ± 0.081 |

Results include free-energy barriers, $W_{peak,calc}$; diffusion coefficients $D_{mem}$ at the membrane center, and $D_{Bulk}$ in aqueous solution); permeabilities, $P$; and contributions to membrane conductance, $G_{ion}$. All uncertainties are represented as the mean ± 1 SE.