

Membrane Permeability from Simulation: Proceed with Some Caution

$$\frac{1}{P_m} = \int_{z_{in}}^{z_{out}} \frac{\exp(w(z)/RT)}{D(z)} dz$$

*inhomogeneous
solubility-diffusion model*

Calculated Data:

$w(z)$ and $D(z)$

Sources of Error:

equilibration, sampling convergence, parameters

z

