

(3,16,17). One of the most easily accessible quantities to monitor in an NPT ensemble is the total area  $A$  of a bilayer with  $N_{\text{chol}}$  cholesterol molecules and  $N_{\text{DPPC}}$  DPPC molecules in each monolayer. One can then define the area per total lipid  $a(x)$  as a function of the mole fraction of cholesterol, defined as  $x \equiv N_{\text{chol}}/(N_{\text{DPPC}} + N_{\text{chol}})$ ,

$$a(x) = \frac{A(x)}{N_{\text{lipids}}} = \frac{A(x)}{N_{\text{DPPC}} + N_{\text{chol}}}. \quad (1)$$

Table 1 and Fig. 1 show that there are some differences between the three simulations, but within statistical error they are rather similar.