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Michal Bachar, Patrick Brunelle, D. Peter Tieleman, and Arvi Rauk*: Molecular Dynamics Simulation of a Polyunsaturated Lipid Bilayer Susceptible to Lipid Peroxidation

Page 7170. Please note that some of the phases of the torsion angles for the potential functions of the *cis,cis*-2,5-heptadiene fragment of polyunsaturated lipids were incorrectly specified in eqs 3, 4, and 6. Additionally, a factor of 2 was omitted from eq 5 and two digits of the first term of eq 6 were interchanged. None of the results and conclusions is affected.

The correct equations are

$$V(\phi_1) = 3.350[1 + \cos(\phi_1 - 180)] -$$

$$1.660[1 + \cos(2\phi_1 - 180)] +$$

$$7.333[1 - \cos(3\phi_1 - 180)]$$
 (3)

$$V(\phi_2) = -5.685 + 7.470[1 + \cos(\phi_2 - 180)] + 3.900[1 + \cos(2\phi_2)] + 1.100[1 + \cos(3\phi_2)]$$
 (4)

$$V(\phi_3) = 0.017308[\phi_3]^2 \tag{5}$$

$$V(\phi_4) = -3.500 + 4.533[1 + \cos(\phi_4 - 180)] + 3.000[1 + \cos(2\phi_4)] + 1.550[1 + \cos(3\phi_4)] + 1.300[1 + \cos(\Theta)]$$
 (6)

where $\phi_1 - \phi_4$ are defined in Figure 1 and Θ is the torsion angle between the vectors defined by the two double bonds, for example, C4–C3 and C6–C7, in the case of *cis,cis*-3,6-decadiene (C10–C9 and C12–C13, in the linoleoate chain). All angles are in degrees and the potential V is in kJ mol⁻¹.

We thank an astute reader for pointing out these errors.

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