ESI

A Multiscale approach to triglycerides Simulations: From atomistic to coarse-grained models and back

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Planarity and Conformation parameters definition

To Analyse molecular conformations, two scalars P and C assessing planarity and conformations, respectively, have been defined. Planarity P is defined as follows:

$$P = \frac{\cos\theta'_{12} + \cos\theta'_{23}}{2} \text{ with:}$$

$$\theta'_{ij} = \begin{cases} \cos\theta_{ij} & \text{if } \cos\theta_{12} \le \frac{\pi}{2} \\ \cos\theta_{ij} - \pi & \text{if } \cos\theta_{12} > \frac{\pi}{2} \end{cases}$$

For each coarse-grained molecule, θ_{ij} are the angles formed by the plane identified by the two peripheral N beads and the extreme C bead of the central tail with those identified by the two peripheral N beads and the extreme C beads of the other two tails (see Fig. S1).

The parameter P belongs to the interval [0,1]: P = 0 means no planar conformation while P = 1 perfectly planar conformation. We choose to consider as planar, those molecules with planarity P exceeding the threshold of 0.8.

The conformational parameter C is defined as follows:

$$C = \frac{\cos\theta_{12} + \cos\theta_{23}}{2} \text{ if P } \square \text{ 1}$$

The parameter C belongs to the interval [-1,1]: C = -1 means *tuning-fork* conformation, C = 0 means *chair* conformation, while C = 1 means *trident* conformation (see Fig. S1). Molecules have been classified as *tuning-forks* if $C \in [-1, 0.8]$, as *chairs* if $C \in [0.2, 0.2]$, as *tridents* if $C \in [0.8, 1]$.

These definitions are easily extended to the atomistic configurations obtained through the backmapping by substituting the coordinates of the N and C beads with the corresponding united atoms coordinates .

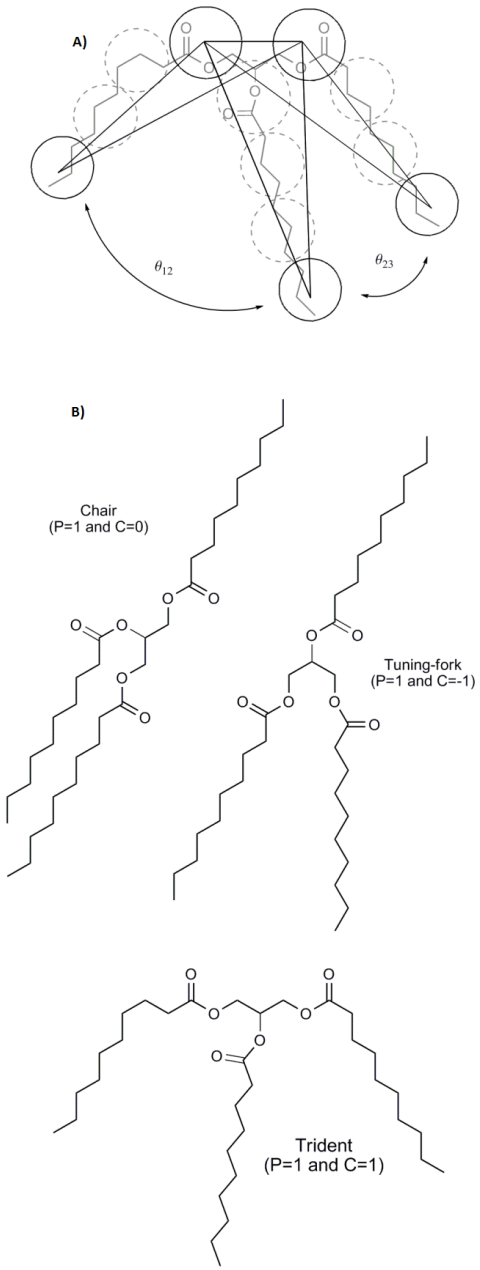

Fig. S1 **A)** θ_{12} and θ_{23} angles used to define planarity P and conformation C. **B)**Structure formulas for tridecanoin related to molecular planar conformations together with P and C values

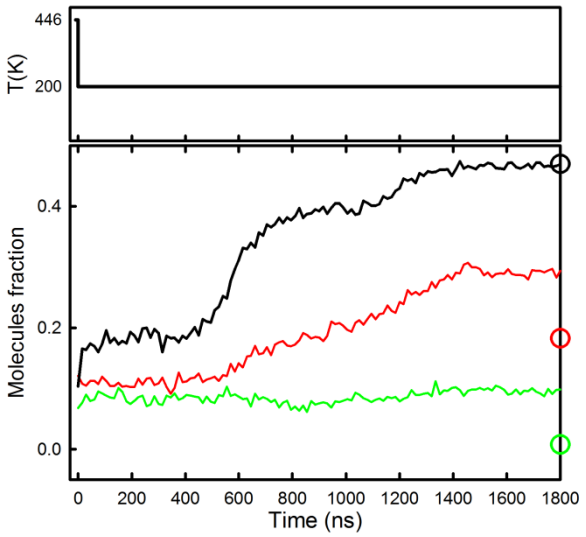

Fig. S2 Time evolution of tuning-fork (black line CG model, black empty circles reverse mapped model), chair (red line CG model, red empty circles reverse mapped model) and trident (green line CG model, green empty circles reverse mapped model) during time for system **CG2**.