[pex39] Self-assembly as predicted by geometric argument

Consider amphiphiles of (effective) volume V in aqueous solution with shapes as sketched in [psl14]. The effective area of their hydrophilic headgroups is a and the length of the their hydrophobic tails is l when fully extended. The dimensionless quantity V/la is a convenient measure to characterize the shape of the amphiphilic molecule between cone-like and cylinder-like. The type of self-assembled structure is the result of balancing two competing agents: (i) the short-range repulsion between particles with shapes, (ii) the efficient shielding of the hydrophobic tails from contact with water. Present an argument that the spontaneous aggregation of amphiphiles into (a) spherical micelles, (b) cylindrical micelles, (c) flat bilayers or vesicles of radius $r \gg l$ is favorable from a pure packing point of view if (a) $V/la \lesssim \frac{1}{3}$, (b) $V/la \lesssim \frac{1}{2}$, (c) $V/la \lesssim 1$, respectively. For spherical and cylindrical micelles (of radius r) the criterion for efficient shielding and mechanical stability is $r \lesssim l$. In a bilayer of width d (flat or forming a vesicle) that same criterion is $d \lesssim 2l$.

Solution: