Effect of Carboxyl Group of Oleic Acid on Polymorphism of Glycine in Water/Oleic Acid Emulsion

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In the specific environment in which water droplets are dispersed in oleic acid, χ – glycine were dominantly produced. In the view of molecular kinetics, the oleic acid molecules could form a layer in which the carboxyl groups are directed into water and the hydrocarbon chains in opposite direction, so that the special binding site of glycine could be generated. To find out the effect of carboxyl functional group of oleic acid on crystallization of glycine, the interaction energy between acetic acid molecules and the various faces of α - and χ -glycine was calculated. The results show that the carboxyl groups are strongly interacted with the surface of χ -glycine and thus those sites are expected to be a favorable growing position of χ -glycine cluster in water solution.