• *Letter to the Editor*

Molecular Dynamics and Glyceride Structure

THERE IS EVIDENCE that the acyloxy groups in the natural depot fats may be distributed in what has been termed the 1,3 random, 2 random pattern (1). According to this pattern the 1- and 3-positions in the glycerol moiety are identical and are occupied by identical kinds and proportions of fatty acyloxy groups distributed at random. The 2-positions may be occupied by the same or a different combination of acyloxy groups also distributed at random. If the combination is the same, the over-all distribution is random; if different, the over-all distribution is non-random.

In the great majority of fats so far examined, if not in all fats, the combination of acyloxy groups occupying the 2-positions differs in kind, proportions, or both from that found in the 1,3-positions,[1] particular groups exhibiting what we will call "specificity"[2] for one or the other location. The over-all distribution is therefore non-random. The degree of specificity may vary greatly from one variety of fat to another, and, usually to a lesser extent, from one sample to another of the same variety.

The kinds and proportions of the acyloxy groups in the 1,3-positions, and the 2-positions, respectively, can be found by means of the pancreatic lipase hydrolysis procedure (1). From these data and with the assumption of 1,3 random, 2 random distribution the percentages of the six molecular varieties SSS, SUS, SSU, USU, UUS, and UUU can be calculated correctly on the basis of probability, at least for fats of the C_{16}–C_{18} chain length variety (1). This is the evidence for the validity of the 1,3 random, 2 random pattern.

Although there is less evidence for their reliability, percentage values for individual triglycerides such as tripalmitin, 2-palmitodiolein, etc. may be calculated in the same way (1). The procedure applies equally well to animal and vegetable depot fats.

If the 1,3 random, 2 random pattern, with some degree of specific orientation, is as common among the natural depot fats as appears likely, it would be of interest and perhaps profitable to know by what mechanism it becomes established. It would seem reasonable to expect it to be the same in all varieties of organism. One such mechanism will be broadly outlined in the following paragraphs.

That the fats stored in living animal tissue are in a state of flux is well known. The subject has been discussed by Shorland (2). In 1951, or earlier, Kartha (3) included a continuous, dynamic, interchange of the acyloxy groups in both animal and vegetable depot fats resulting from the reversible action of lipases, as part of a mechanism, based on probability, by which ordered patterns of triglyceride molecules may be formed *in vivo*. He assumed no preferential associations between acyloxy groups and glyceryl positions.

Stein (4) has indicated that there is rapid mixing of newly synthesized triglycerides with those already present in the epididymal fat pads of the rat. Such mixing could occur rapidly by interesterification, by rapid hydrolysis and resynthesis, or by combinations of such processes. Frequent and repeated migration of the acyloxy groups in depot fats from one to another glyceryl carbon in the same or another molecule would under the following circumstances result in orderly patterns of distribution.

If the 1- and 3-positions of the glycerol moiety are identical, they will be occupied at any instant by identical kinds and proportions of acyloxy groups. Specific varieties of acyloxy groups may, conceivably, enter a 2-position more readily than a 1- or 3-position, or having entered it may leave it less readily. In such or similar case they will, at any instant, occupy it in greater-than-random proportions and will exhibit specificity for that position. Other groups may show a degree of specificity for the 1- and 3-positions, and still others may exhibit no specificity at all.

The 1- and 3-positions will then, at any instant, be occupied by identical kinds and proportions of acyloxy groups. The 2-positions will be occupied by another combination of groups. Those present in each position will be distributed therein at random provided that occupancy by any group of any particular position in a molecule is independent of what occurs in the other two positions. The circumstance may perhaps be more likely to exist in reactions controlled by enzymes.

If this assumption is correct the acyloxy groups are distributed in the 1,3 random, 2 random pattern with some degree of specific orientation to either the 2- or 1,3-positions, which is the end the proposed mechanism was to achieve. The same mechanism would result in over-all random distribution if there were no specificity factor involved.

The proposed mechanism is a way in which triglycerides, newly appearing in the depot fat, could be quickly incorporated into the patterns of acyloxy distribution and specificity peculiar to the depot, regardless of their original structural composition. It contains the element of chance which makes it possible to calculate structural composition on the basis of probability.

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[Received March 14, 1962—Accepted February 18, 1963]

[1] The term "1,3-positions" denotes the 1- and 3-positions jointly. In 1,3 random, 2 random distribution the percentage composition is identical for the 1-, 3-, and 1,3-positions.

[2] It should be noted that in 1,3 random, 2 random distribution, specificities for the 1-positions will be identical with those for the 3-positions.