Technical

Computer Determination of All Individual Structures of Triglyceride Molecules of Fats and Oils: II

V. KOMAN, Lipid Laboratory, CHTF, Slovak Polytechnik University, Bratislava, Czechozlovakia, J. KOTUČ, and M. CSICSAYOVÁ, ÚVT VŠ, Comenius University, Bratislava, Czechoslovakia

ABSTRACT

Computer determination of all the individual structures of triglyceride molecules (ISTM) with respect to the present criteria as well as the number of double bonds in triglyceride molecules of fats and oils is described. In addition to the transformation of the combinational AAA . . . . ABC types of triglyceride molecules into their corresponding ISTM, the ISTM can also be obtained from the aligned sum SSS . . . . UUU structural types of triglyceride molecules of fats and oils.

INTRODUCTION

The number of possible structural forms of triglyceride molecules of fatty oils is very great in relation to the number of fatty acids present.

The answers to the questions regarding the number of triglyceride structures in relation to the experimentally determined number of fatty acids, especially their placement in C-1,3 and C-2 positions in triglyceride molecules, are relatively difficult (1,2). A very advantageous method for a more exact solution of the above complex of structural questions for fatty oil triglyceride molecules seemed to be the application of combined stereospecific pancreatic lipolysis with adsorption and partition chromatography and progressive computer techniques (3-5).

Another problem in the sphere of the structure of triglyceride molecules is the method of interpreting the ionic structure. The following forms of interpretation seem to be suitable:

1. With the help of the six forms of aligned sums of SSS . . . . UUU triglyceride structures, in which fatty acids are considered only in terms of their cumulated saturated (S) and unsaturated (U) but otherwise unnamed forms. Up to the present, the majority of results investigating the structures of triglyceride molecules have been interpreted in this way.
2. With the help of individual TG structure forms, by transformation of all combinational mono- (AAA), di- (AAB . . . .), and tricomponent (ABC . . . .) types by replacement with specific fatty acids with respect to their qualitative-quantitative and positional parameters.
3. With the help of triglyceride structure forms of molecules according to the number of double bonds (4,6,7).
4. With the help of individual structures of triglyceride molecules formed by transforming aligned SSS . . . . UUU types with the help of individual experimentally determined fatty acids respecting all their qualitative-quantitative and positional parameters.

A method for determining all ISTM of fats and oils using the criteria under point 2 and under point 1, differentiating individual fatty acids in positions C-1,3 and C-2 in triglyceride molecules of maize oil and rapeseed oil, has been described in a previous paper (5).

The aim of this work was to elaborate materials for testing the possibility of computer determination of all ISTM with fatty acids positionally differentiated according to the criteria under points 3 and 4.

EXPERIMENTAL PROCEDURES

Samples

Maize oil, whose data concerning the composition-position of individual fatty acids were taken from Vander Wal (8) and compared with Hayakawa's results (9), was used as a model. As input data for rapeseed oil determination, we used the same qualitative-quantitative and position data which were experimentally obtained under conditions of stereospecific lipolysis, thin layer chromatography and gas liquid chromatography rations as described previously (5).

Conditions for Program Construction

The computer program for the determination of individual structures of triglyceride molecules by the development of particular aligned SSS . . . . UUU structural types forms an additional part of the program which has been described previously. It is a two-step program. In the first step, the main criteria are the presence and/or absence of double bonds in each of the experimentally determined or entering fatty acids. In step two, the main criterion is the total number of double bonds in the appropriate triglyceride molecules. The representation of fatty acids for organizing ISTM into the corresponding groups according to the present criteria and number of double bonds, as well as for the whole operating process and output print, are the forms "$C_{x:0}$" and "$C_{x:n}$", where x represents the number of carbon atoms in the chain of the fatty acid under investi-

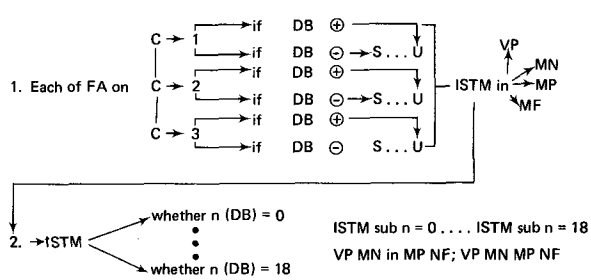

FIG. 1. Program conditions for determining ISTM by development of aligned SSS . . . . UUU structures. Abbreviations: FA = fatty acid; DB = double bond; S = saturated, U = unsaturated; ISTM = individual structures of triglyceride molecules; VP = weight percentage; MN = mol number; MP = mol percentage; MF = mol fraction; n(DB) = number of double bonds.

TABLE I

Computer Output Showing All Determined Individual Structures of Particular Alignment Types of Maize Oil Triglyceride Molecules

Number	Positions of individual fatty acids C_1	C_2	C_3	Weight (%)	Mol value	Mol (%)
	S	S	S	0.000	0.000	0.000
	S	S	U	0.000	0.000	0.000
	U	S	U	0.000	0.000	0.000
	S	U	S			
1	16:0	18:2	16:0	2.268	0.027	2.049
2	16:0	18:1	16:0	0.972	0.012	0.878
3	16:0	18:2	18:0	0.781	0.010	0.706
4	16:0	18:1	18:0	0.335	0.004	0.303
4	Sums			4.356	0.053	3.936
	U	U	S			
1	18:2	18:2	16:0	12.424	0.145	11.226
2	18:1	18:1	16:0	2.884	0.034	2.606
3	18:2	18:1	16:0	5.334	0.078	7.890
4	18:2	18:1	18:0	0.917	0.011	5.040
5	18:3	18:2	16:0	0.227	0.304	0.304
6	18:1	18:2	16:0	6.728	0.078	3.509
7	18:1	18:2	18:0	1.159	0.014	2.100
8	18:3	18:2	16:0	0.336	0.004	1.903
9	18:2	18:2	18:0	2.140	0.025	1.933
10	18:1	18:1	18:0	0.497	0.006	0.449
10	Sums			32.646	0.398	36.960
	U	U	U			
1	18:2	18:2	18:2	17.013	0.193	17.532
2	18:1	18:1	18:1	2.139	0.024	2.188
3	18:1	18:1	18:2	7.898	0.089	8.100
4	18:2	18:2	18:3	0.621	0.007	0.642
5	18:1	18:1	18:3	0.144	0.002	0.138
6	18:1	18:2	18:1	4.990	0.056	4.509
7	18:2	18:3	18:2	0.122	0.001	0.110
8	18:2	18:2	18:1	18.428	0.209	16.652
9	18:2	18:1	18:2	7.291	0.083	8.589
10	16:0	18:2	18:3	0.227	0.003	0.241
11	18:1	18:3	18:2	0.132	0.001	0.119
12	18:3	18:1	18:2	0.266	0.003	0.274
12	Sums			59.271	0.671	59.094
26	Sums	Total		96.273	1.122	99.990

gation and can be in the range from 0 to 30, and n expresses the number of double bonds, in the range from 0 to 6 for a given fatty acid, or from 0 to 18 for a given triglyceride molecule. The printout format contains the ISTM determined under these conditions printed in two separate tables and in all concentration expressions. The program conditions for ISTM computing by the development of aligned SSS . . . . UUU type structures are illustrated in Figure 1.

Fatty acids positions C-1 and C-3 are also in this case quantitatively and qualitatively considered to be the same or undifferentiated.

The whole program in its final version was reimplemented for use on the SIEMENS model 4004/150 computer. The programming language was again FORTRAN IV.

RESULTS AND DISCUSSION

To compare the ISTM results, we have again used maize oil as a model. The following are the summary values of alignment SSS . . . . UUU types of triglyceride molecules, obtained under calculation conditions described above (in weight percentage): SSS = 0.00%, SUS = 4.74 %, SSU = 0.00%, USU = 0.00%, UUS = 32.6141%, and UUU = 59.4318%. ISTM results obtained under the previously described figure by the development of these aligned structures and the replacement of S and U symbols with individual fatty acids with respect to their C-1,3 and C-2 positions are given in Table I. We have given the results for ISTM maize oil in an unabbreviated form. From the results

TABLE II

Individual Structures of Triglyceride Molecules of Maize Oil Grouped with Respect to the Sum Number of Double Bonds

No. of double bonds	ISTM Fatty acids position C_1	C_2	C_3	Weight (%)	Mol value	Mol (%)
n = 0	—	—	—	0.000	0.000	0.000
n = 1	16:0	18:1	16:0	0.972	0.012	0.878
	16:0	18:1	18:0	0.335	0.004	0.303
	16:0	18:2	16:0	2.268	0.027	2.049
n = 2	18:1	18:1	16:0	2.884	0.034	2.606
	18:1	18:1	18:0	0.497	0.006	0.449
	16:0	18:2	18:0	0.781	0.010	0.706
	18:1	18:1	18:1	2.139	0.024	2.188
n = 3	16:0	18:1	18:2	5.334	0.078	7.890
	18:0	18:1	18:2	0.917	0.011	5.040
	16:0	18:2	18:1	6.728	0.078	3.509
	18:0	18:2	18:1	1.159	0.014	2.100
n = 4	18:1	18:1	18:2	7.898	0.089	8.100
	18:1	18:2	18:1	4.990	0.056	4.509
	18:2	18:2	16:0	12.424	0.145	11.226
	18:2	18:2	18:0	2.140	0.025	1.933
	18:1	18:1	18:3	0.144	0.002	0.138
n = 5	18:2	18:2	18:1	18.428	0.209	16.652
	18:2	18:1	18:2	7.291	0.083	8.589
	16:0	18:2	18:3	0.227	0.003	0.304
	16:0	18:2	18:3	0.227	0.003	0.241
n = 6	18:2	18:2	18:2	17.013	0.193	17.532
	18:1	18:2	18:3	0.336	0.004	1.903
	18:1	18:3	18:2	0.132	0.001	0.119
	18:3	18:1	18:2	0.266	0.003	0.274
n = 7	18:2	18:2	18:3	0.621	0.007	0.642
	18:2	18:3	18:2	0.122	0.001	0.110

in Table I we can see that after transforming the aligned summary structures of maize oil into their individual forms by suitable computing methods, we have again obtained all of the fully defined structure forms.

Table II contains the maize oil ISTM results obtained under the described conditions and listed according to the number of double bonds in triglyceride molecules, likewise in the unabbreviated form of computer printout.

Summary results of aligned triglyceride structures of rapeseed oil, whose composition and position data regarding fatty acids followed from experimental results, were as follows: SSS = 1.4704%, SUS = 4.0615%, SSU = 9.5625%, USU = 15.5471%, and UUU = 42.9448%. By expanding these results and transforming the S and U terms of all individual rapeseed oil fatty acids using the described method, we have also obtained the whole table of ISTM. It is in the same form as the table for maize oil, but due to the number of determined rapeseed oil fatty acids is much larger and has been omitted. The results for rapeseed oil will be treated in a separate work summarizing all the ISTM results for natural and treated samples as well as for fats and oils taken from both normal and pathological tissues. It is worthwhile for rapeseed oil to give at least the numbers of ISTM obtained using the following criteria:

1. With and without double bonds.
2. With the number of double bonds in triglyceride molecules.

In the first case, we have the following results: SSS has 0 ISTM, SSU has 11 ISTM, SUS has 5 ISTM, USU has 38 ISTM, UUS has 17 ISTM, and UUU has 71 ISTM. In the second case, that is, using the criterion of the number of double bonds in triglyceride molecules, we have the following values in the case of rapeseed oil: when n = 0, rapeseed oil contains no ISTM; when n = 1, ISTM = 16; when n = 2, ISTM = 54; when n = 3, ISTM = 39; when n = 4, ISTM = 23; when n = 5, ISTM = 10.

It is interesting that in the case of maize oil, ISTM were obtained with a maximum of 7 double bonds while for rapeseed oil the maximum is only 5 double bonds. All the

ISTM results for rapeseed oil given in Tables I and II are quantitatively, qualitatively, and positionally analogous with the result form on the computer output part.

In the course of this work we have added subroutine to the program for deducing all the ISTM of fats and oils which utilizes the equations for fatty acid calculation giving the third positional value if total C-1,2,3 and C-2 or C-1,3 fatty acids are known. According to Vander Wal (2) those equations are: C-2 = 3 (C-1,2,3)- 2 (C-1,3)or C-1,3 = 3 [(C-1,2,3)-(C-2)] /2. Thus it will be possible to calculate the data regarding fatty acids on appropriate positions and in this way to determine the relevant correlation coefficient between experimental and computed results in composition and presence of individual fatty acids in triglyceride molecules of fats and oils.

From the combined results obtained when using maize oil as a model and rapeseed oil as an experimental subject described in this and the previous paper (5), it is possible to get a complete picture of the capabilities of the computer program which is now completed for the purpose of defining and interpreting all ISTM, both from mono-, di-, and tricomponent AAA . . . . ABC molecular types as well as from that of the aligned SSS . . . . UUU structural types, further extended by the differences according to the presence or absence of all saturated and unsaturated fatty acids and grouped in the final phase according to the number of double bonds of single triglyceride molecules in fatty oil samples that were under observation.

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