Jaocs News Feature

Suggestions on nomenclature of acylglycerols (glycerides)[1]

ROBERT G. JENSEN, Department of Nutritional Sciences,
University of Connecticut, Storrs, Connecticut 06268

INTRODUCTION

The report by the International Union of Pure and Applied Chemistry (IUPAC)-International Union of Biochemistry (IUB) Commission on Biochemical Nomenclature, entitled the "Nomenclature of Lipids" (1) explains the necessity for semisystematic names in the field of lipids and they propose the rules discussed below.

LIPIDS CONTAINING GLYCEROL

Individual Compounds

In designating esters, ethers, and other O-derivatives of glycerol, rules 10 and 11 of the "Rules of Carbohydrate Nomenclature" (2) are followed. These rules provide that: (A) if the hydrogen atom of an alcoholic hydroxyl group is replaced by another atom or group, the name of the parent compound may be retained as the root of the substituted compound and that, in such names, the prefix (denoting the substitutent) is attached directly to the root; and (B) an ester may be named by placing after the unchanged name of the parent compound, and separated therefrom by a space, the appropriate numeral (indicating position) and a hyphen, as prefix to the name of the anionic group derived from an acid.

If the substitution is on the carbon atom, the compound is designated by its systematic name and not as a derivative of glycerol. It is permissible, therefore, to omit the symbol "O" if the substitution is on the oxygen atoms of glycerol.

Examples: Glycerol tristearate, or tristearoylglycerol, or tri-O-stearoylglycerol; 1,3-benzylideneglycerol or 1,3-O-benzylideneglycerol; glycerol 2-(dihydrogen phosphate) (a permissible alternative to this term is "glycero-2-phosphoric acid").

To designate the stereochemistry of glycerol derivatives, the carbon atoms of glycerol are numbered stereospecifically. The carbon atom that appears on top in the Fischer projection that shows a vertical carbon chain with the secondary hydroxyl group to the left is designated as C-1. To differentiate such numbering from conventional numbering conveying no steric information, the prefix "*sn*-" (for stereospecifically numbered) is used. This term is printed in lower case italics, even at the beginning of a sentence, and it immediately precedes the term signifying glycerol and is separated from it by a hyphen. The prefix "*rac*-" (for racemo) precedes the full name, if the product is an equal mixture of both antipodes, and the prefix "X-," if the configuration of the compound is either unknown or unspecified.

Examples: *sn*-Glycerol 3-(dihydrogen phosphate) or *sn*-glycero-3-phosphoric acid for the stereoisomer previously known as either L-α-glycerophosphoric acid (3) or as D-glycerol 1-phosphate (4) *rac*-1-hexadecylglycerol; X-glycerol 1,2-dipalmitate 3-stearate.

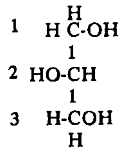
In addition to these, the following comments and modifications are offered in the paragraphs below.

Acylglycerols is preferred for neutral fats, eg. triacylglycerol, etc.

When the substitutent is known, it is identified by an acceptable systematic or common name and located by number, not English or Greek letters. The word glycerol should be first in sequence. Since some of the names can be long and awkward, it is suggested the following shorthand be used in publications after an initial explanation: glycerol tristearate, 18:0-18:0-18:0; glycerol-1-stearate-2-oleate-3-palmitate, 18:0-18:1-16:0.

In this system, it is understood that numbering is from left to right. 18:1 is *cis*-9-oleic, 18:2 is *cis,cis* 9,12 linoleic, etc. Other acids are identified as follows: eg. elaidic acid 18:1-t, petroselenic acid 18:1-6, etc., staring with the functional group closest to the carboxyl. Enantiomeric glycerides are prefixed by *sn*-. If the composition is unknown or unspecified, the prefix X- is used. If the composition of the 2 position is known, but the stereoconfiguration of the 1 and 3 positions is not, for example, as from a pancreatic lipolysis of a natural fat, then the prefix is β. In these circumstances, the 1 and 3 positions could contain mixtures of enantiomers and racemates.

To designate stereospecificity, the glycerol molecule is drawn with the secondary hydroxyl to the left and the other two to the right. The hydroxyl above the secondary hydroxyl is number 1, etc.



$$\begin{array}{ll} 1 & \overset{H}{HC}\text{-OH} \\ & | \\ 2 & \text{HO-CH} \\ & | \\ 3 & \underset{H}{\text{H-COH}} \end{array}$$

For example, lecithin becomes *sn*-3-phosphatidyl choline. This system is quite arbitrary but is easily understood and recognizable. A major advantage is that there are no apparent changes in structure due to changes in the nature of the acyl groups as with the Cahn-Ingold-Prelog system. This will be discussed below.

These further suggestions are elaborations of the IUPAC-IUB rules. The *sn*-nomenclature, as presently used, arose from a decision by Hirschmann (5) to give the lower number 1 to prochiral S (A in the reference). Hirschmann and Hanson (6) subsequently recommended that *pro* R precede *pro* S as being consistent with other established priorities. If this recommendation is applied to glycerol derivatives, the earlier *sn*-nomenclature would be reversed. Recognizing the confusion that would result, Hirschmann and Hanson (7) specifically excluded glycerol from their recommendation. There is precedent for using special numbering for local systems. Thus, the original *sn*-numbering for glycerol will be retained.

Ideally, all lipid chemists and biochemists should become familiar with and use the Cahn-Ingold-Prelog R and

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[1] This paper is part of the nomenclature program of the AOCS Nomenclature Subcommittee.

TABLE I

Racemic Acylglycerols[a]

Systematic name	Shorthand
Glycerol-1-palmitate	16:0-OH-OH
Glycerol-1,2-dipalmitate	16:0-16:0-OH
Glycerol-1-palmitate-2-oleate	16:0-18:1-OH
Glycerol-1,3-dipalmitate	16:0-OH-16:0
Glycerol-2-palmitate	OH-16:0-OH
Glycerol-1-oleate-2,3-dipalmitate	18:1-16:0-16:0

[a] Absence of prefix signifies racemic or RS. These will be observed almost altogether only with synthetic compounds.

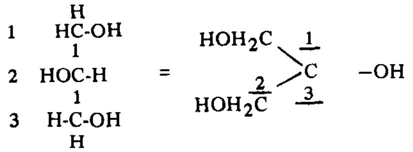
TABLE II

Enantiomeric Acylglycerols

Systematic name	Shorthand	CIP[a]
sn-Glycerol-3-palmitate	*sn*-OH-OH-16:0	R
sn-Glycerol-1-palmitate	*sn* 16:0-OH-OH	S
sn-Glycerol-1,2-dipalmitate	*sn* 16:0-16:0-OH	S
sn-Glycerol-2,3-dipalmitate	*sn* OH-16:0-16:0	R
sn-Glycerol-1-palmitate-2-oleate	*sn* 16:0-18:1-OH	S
sn-Glycerol-1-oleate-2-palmitate	*sn* 18:1-16:0-OH	S
sn-Glycerol-1-palmitate-3-oleate	*sn* 16:0-OH-18:1	R
sn-Glycerol-1-oleate-3-palmitate	*sn* 18:1-OH-16:0	S
sn-Glycerol-1-palmitate-3-stearate	*sn* 16:0-OH-18:0	R
sn-Glycerol-1-oleate-3-stearate	*sn* 18:1-OH-18:0	S
sn-Glycerol-1-palmitate-3-myristate	*sn* 16:0-OH-14:0	S
sn-Glycerol-1,2-dipalmitate-3-oleate	*sn* 16:0-16:0-18:1	R
sn-Glycerol-1-oleate-2,3-dipalmitate	*sn* 18:1-16:0-16:0	S
sn-Glycerol-1,2 distearate-3-oleate	*sn* 18:0-18:0-18:1	R
sn-Glycerol-1,2 distearate-3-elaidate	*sn* 18:0-18:0-18:1^t	S
sn-Glycerol-1,2 dielaidate-3-oleate	*sn* 18:1^t-18:1^t-18:1	R
sn-Glycerol-1,2 dioleate-3-linoleate	*sn* 18:1-18:1-18:2	R
sn-Glycerol-1-laurate-2-myristate-3-palmitate	*sn* 12:0-14:0-16:0	R

[a] CIP = Cahn-Ingold Prelog system.

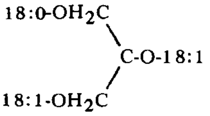
S system, so as to have a universal nomenclature. For an application of this system to acylglycerols see the paper by Schlenck (8).



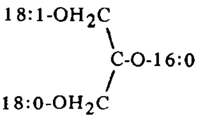
To determine whether an acylglycerol is R (rectus) clockwise or S (sinister) counterclockwise, Schlenck turns the molecule so that it resembles a three spoke steering wheel with the H on carbon-2-beneath the plane of the paper. Then arbitrarily place the secondary OH or substitutent group to the right and the other two groups at upward and downward angles with 1 on top. The priority of the groups then is determined from the list below. 2 Position OH, OCR, and OCOR take precedence over 1 or 3 position in which the priority is $CH_2OCOR > CH_2OCR > CH_2OH > H$.

Longer chains precede shorter chains, two double bonds precede one, *cis*-precedes *trans*-, and a branched chain precedes an unbranched chain.

Then starting with the highest priority group, OH, the direction of decrease in the order of priority is determined. If clockwise, it is R; if counterclockwise, it is S. If, as in the case of glycerol, substitution at one of the -CH_2OH groups leads to S chirality then the -CH_2OH group is prochiral S or *pro*-S. Two examples are shown below. Ester bonds are assumed.



Triacylglycerol 1



Triacylglycerol 2

By present nomenclature, triacylglycerol 1 is *sn*-glycerol-1-stearate-2, 3-dioleate. It is also R, because, starting with the highest priority 18:1-ester at carbon 2, the next highest group is -CH_2O-18:1 and the least -CH_2O18:0. The direction of decreasing priority is, therefore, clockwise, and the molecule is R. Since triacylglycerol 2 is *sn*-glycerol-1-oleate-2-palmitate-3-stearate, the direction of decreasing priority is counterclockwise and the molecule is S. With triacylglycerols, the highest priority group is always on carbon 2, because this will be -OCOR which takes precedence over -CH_2OR. The type of acyl group does not matter. However, if some group other than hydrogen were attached directly to the 2 position, this position might not take precedence over 1 or 3.

As indicated above, while R and S do convey the stereochemical configuration of the acylglycerol, annoying "false inversions" can occur. If the stearate in triacylglycerol 1 is changed to linoleate, then the molecule becomes S, because 18:2>18:1 and the direction of decreasing priority becomes counterclockwise or S. This is a minor annoyance and should not deter lipid chemists from using R and S nomenclature, as the primary acyl groups are located readily in terms that all organic chemists should be able to understand. A list of examples with comments is given in Tables I and II.

Note that all 1,2-*sn*-diacylglycerols are S and conversely 2,3 s are R. The 1,3-*sn*-diacylglycerols change according to the acyl group, as do the triacylgycerols. If the highest priority acyl group is in the 1 position, the designation is S. If in the 3 position, it is R. Again the group with highest priority is always on the 2 carbon; -OH or -OCOR.

The stereochemical configuration of synthetic acylglycerols can be designated by either *sn*- or the RS system. However, the RS system cannot be applied to natural fats which may be mixtures of racemic and enantiomeric triacylglycerols, unless individual triacylglycerols are separated. In these cases, the *sn*-system can be used. For example, a Brockerhoff stereospecific analysis of a triacylglycerol mixture identifies the acids in *sn*-positions 1, 2, and 3 because of the stereospecificity of phospholipase A_2. R or S cannot be applied because position 1 and 3 contain mixtures of acids. To summarize, R and S can be used only with pure synthetic or isolated individual enantiomeric acylglycerols. The present *sn*-system is applicable both to these and to natural fats, and its use is recommended highly.

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