The Nomenclature of Lipids¹

Recommendations (1976)^{2,3}

IUPAC-IUB Commission on Biochemical Nomenclature⁴

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In 1967, a "Document for Discussion" on lipid nomenclature (1) was issued by CBN. It included a special system for the designation of configuration in glycerol derivatives that deviated considerably from standard sterochemical nomenclature. This system is based upon a fixed numbering ("stereospecific numbering") for glycerol, regardless of substituents. It was hoped (1) that "discussion will lead shortly to the formulation" of recommendations acceptable to chemists in the field of lipids.

In subsequent years, there has been little discussion about this principle of stereospecific numbering; it has been well-accepted within the field of glycerol derivatives, for which it has been especially useful,⁵ and is widely used. However, during this same period, many new and complex lipids and glycolipids have been

isolated. Moreover, the Commissions on the Nomenclature of Organic Chemistry (CNOC) and Inorganic Chemistry (CNIC) issued, in 1973, "Nomenclature of Organic Chemistry, Section D" (2), which includes a section on the nomenclature of phosphorus-containing organic compounds and necessitates a reconsideration of the earlier nomenclature (1) in this area.

The present "Recommendations 1976" are based on reports of working groups on lipids⁶ and glycolipids.⁷ The main features are:

- 1. the system of stereospecific numbering is retained;
- 2. semisystematic nomenclature is extended to the plasmalogens;
- 3. a semisystematic nomenclature for higher glycosphingolipids, based on trivial names for specific tri- and tetrasaccharides, is proposed.

¹Document² of the IUPAC-IUB Commission on Biochemical Nomenclature (CBN) approved by IUPAC and IUB in 1976, and published with the cooperation of the IUB Commission of Editors of Biochemical Journals.³ Comments on these Recommendations and suggestions for future revisions may be sent to any member of CBN.⁴

²These Recommendations are a revision and extension of "The Nomenclature of Lipids," which appeared in 1967, as amended in 1970 (1).

³Reprints of this document, supplied by the publishing journals, may be obtained from W.E. Cohn (Director of the NAS-NRC Office of Biochemical Nomenclature), Biology Division, Oak Ridge National Laboratory, Box Y, Oak Ridge, Tennessee, U.S.A. 37830.

⁴Members of CBN are: O. Hoffmann-Ostenhof (Chairman), W.E. Cohn (Secretary), A.E. Braunstein, H.B.F. Dixon, B.L. Horecker, W.B. Jakoby, P. Karlson, W. Klyne, C. Liébecq, E.C. Webb.

⁵CBN does not wish to imply that the idea of stereospecific numbering should be applied to other groups of compounds. It is the symmetry of glycerol itself, but the asymmetry of its derivatives carrying different substituents at O-1 and O-3, as well as the unique place of these compounds in lipid metabolism, that makes this special treatment desirable.

⁶Members of the Working Group on Lipid Nomenclature: H. Hirschmann (U.S.A.), P. Karlson (Germany; convenor), W. Stoffel (Germany), F. Snyder (U.S.A.), S. Veibel (Denmark), F. Vögtle (Germany).

⁷Members of the Working Group on Glycolipid Nomenclature: S. Basu (U.S.A.), R.O. Brady (U.S.A.), R.M. Burton (U.S.A.), R. Caputto (Argentina), S. Gatt (Israel), S.I. Hakomori (U.S.A.), M. Philippart (U.S.A.), L. Svennerholm (Sweden), D. Shapiro (Israel), C.C. Sweeley (U.S.A.), H. Wiegandt (Germany; convenor).

RECOMMENDATIONS

I. FATTY ACIDS, NEUTRAL FATS, LONG-CHAIN ALCOHOLS AND LONG-CHAIN BASES

A. Generic Terms

Lip 1.1 The term "fatty acid" designates any one of the aliphatic monocarboxylic acids that can be liberated by hydrolysis from naturally occuring fats and oils. In the terms "free fatty acids" or "nonesterified fatty acids," now widely in use, "free" and "nonesterified" are actually redundant and should be omitted (See Lip. 1.14). [The designation "aliphatic carboxylate (C_{10} · C_{26} , nonesterified)" used by the Commission on Quantities and Units in Clinical Chemistry is correct, but rather cumbersome.] Whenever the *sum* of fatty acids and their esters is determined by an analytical method, this should be explicitly stated. (See also Lip 1.6).

Lip 1.2 "Neutral fats" are mono-, di-, or triesters of glycerol with fatty acids, and are therefore termed monoacylglycerol, diacylglycerol, or triacylglycerol, as appropriate. "Acylglycerols" includes mixtures of any or all of these.

Comments. i) The term "acyl" is used in Organic Nomenclature (3) to denote the radical formed by loss of the OH group from the acid function of any acid (cf. Lip 1.6). We are concerned here with acyl radicals of aliphatic carboxylic acids with four or more carbon atoms, the larger members of which (> C_{10}) are also known as "higher fatty acids."

ii) The old terms monoglyceride, diglyceride, and triglyceride are discouraged and should progressively be abandoned, not only for consistency, but mainly because strict interpretation does not convey the intended meaning. "Triglyceride," taken literally, indicates three glycerol residues (e.g., cardiolipin), diglyceride two (e.g., phosphatidylglycerol), and a monoglyceride is a monoacylglycerol.

Lip 1.3 The generic term "long-chain alcohol" or "fatty alcohol" refers to an aliphatic compound with a chain-length greater than C_{10} that possesses a terminal CH₂OH group. Such alcohols should be named according to systematic nomenclature (3). (See Lip 1.7).

Lip 1.4 The term "sphingoid" or "sphingoid base" refers to sphinganine (cf. Lip 1.8), [Derythro-2-amino-1,3-octadecanediol (I)], to its homologs and stereoisomers (II,III), and to the hydroxy and unsaturated derivatives of these compounds (IV-VI). The term "long-chain base" may be used in a wider sense to indicate any base containing a long-chain aliphatic radical. Lip. 1.5 The following generic terms are used for the following groups of compounds:

- (a) **sphingolipid**, for any lipid containing a sphingoid;
- (b) ceramide, for an N-acylated sphingoid;
- (c) sphingomyelin, for a ceramide-1-phosphocholine. (See ref. 2 for this use of "phospho"; also Lip 2.11);
- (d) glycosphingolipid, for any lipid containing a sphingoid and one or more sugars. (See sections I,B,2 and II,A for other generic terms).

B. Individual Compounds

1. Fatty acids and alcohols.

Lip 1.6 Fatty acids (cf. Lip 1.1) and their acyl radicals (cf. Lip 1.2, comment i) are named according to the IUPAC Rules for the Nomenclature of Organic Chemistry (ref. 3, Rule C-4). (A list of trivial names is given in Appendix A.) Fatty acids are numbered with the carbon atom of the carboxyl group as C-1. By standard biochemical convention, the ending "-ate" in, e.g., palmitate denotes any mixture of the free acid and its ionized form in which the cations are not specified. The ending "-ate" is also used to designate esters, e.g., cholesteryl palmitate, ethylidene dilaurate, etc. (cf. Lip 1.12). Structural isomers of polyunsaturated acids, hitherto distinguished by Greek letters (e.g., α - and γ linolenic acids), are better distinguished by the locants of the unsaturated linkages [e.g., (9,12,15)- and (6,9,12)-linolenic acids, respectively]. (See Lip 1.15). However, the Greek letter prefixes may be useful in (defined) abbreviations (see Appendix A).

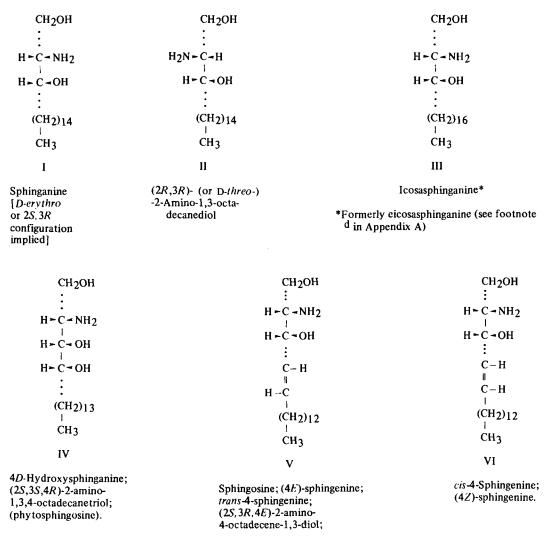
Lip 1.7 Long-chain alcohols (fatty alcohols) and the radicals derived from them should be designated by their systematic names (ref. 3, Rules C-201 and A-1 et seq.), but not by trivial names that are derived from those of fatty acids.

Examples:

- 1-hexadecanol and hexadecyl-, not palmityl alcohol and palmityl-;
- 1-dodecanol and dodecyl-, not lauryl alcohol and lauryl-.

2. Sphinganine and derivatives.

Lip 1.8 The compound previously known as dihydrosphingosine [2D-amino-1,3D-octadecanediol or D-erythro-2-amino-1,3-octadecanediol or (2S, 3R)-2-amino-1,3-octadecanediol] is called sphinganine (I).



Lip 1.9 Trivial names of higher or lower homologs of sphinganine may be derived by adding a prefix (ref. 3, Rule A-1) denoting the total number of carbon atoms in the main chain of the homolog, e.g., icosasphinganine* for the C_{20} compound (III), hexadecasphinganine for the C_{16} compound.

Lip 1.10 Affixes denoting substitution of sphinganine (hydroxy, oxo, methyl, etc.) are used as usual, according to existing rules (3). The configurations of additional substituents should be specified by the prefixes "D" or "L" (italic capitals, cf. ref. 4) following the locant of substitution. These prefixes refer to the orientation of the functional groups to the right or left, respectively, of the carbon chain when

written vertically in a Fischer projection with C-1 at the top (cf. Formulae I-VI). If the configuration is unknown, the prefix "X" may be used. In the case of a racemic mixture, "rac" should be used as a prefix to the name.

Sphingoids differing from sphinganine in their configurations at C-2 and/or C-3 should be named *not* as derivatives of sphinganine, but with fully systematic names (3), using the prefixes D-threo, L-erythro, as appropriate, e.g., D-threo-2-amino-1,3-octadecanediol, or (2R, 3R)-2-amino-1,3-octadecanediol, for II (cf. Rule Carb-8 in ref. 5). (Cf. Lip 1.11, ex. 4).

Comments. i) The semisystematic names for the sphingoids are significantly shorter than the fully systematic names only if the terms chosen imply not only substituents but also configurations. Therefore, the name "sphinganine" specifies the D-erythro configuration, and it is

^{*}See footnote d in Appendix A re "icosa" for "eicosa."

logical that the names of stereoisomers of sphinganine differing in configuration at C-2 and/or C-3 should not include "sphinganine" as a root. [This recommendation differs from that in the previous document (1).]

ii) The configurations usually encountered have identical configurational prefixes only if a D/L but not if the R/S system (6) is used; e.g., C-3 is D and R in icosasphinganine (III) and D and S in 4D-hydroxysphinganine (IV). Whenever it is desirable to use the R/S system, the fully systematic name should be used with the specification of configuration at every center (and, when applicable, of the configuration at the double bond).

Examples:

(2R,3R)-2-amino-1,3-octadecanediol, for II;

(2S,3S,4R)-2-amino-1,3,4-octadecanetriol

for IV;

(2S,3R,4E)-2-amino-4-octadecene-1,3-diol for sphingosine (V) (See also Lip 1.11).

Lip 1.11 Names for unsaturated compounds are derived from the names of the corresponding saturated compounds by the appropriate infixes, namely ene, diene, yne, etc. (3). If the geometry of the double bond is known, it should be indicated by the more modern E-Zsystem (cf. 6, Rule E-2.2), e.g., (4E)-sphingenine for sphingosine (V).

Comment. The trivial name "sphingosine" (V) is retained. If trivial names other than sphingosine are used, they should be defined in each paper in terms of this nomenclature, or of the general nomenclature of organic chemistry (3).

Other names for compounds described in Lip 1.10 and 1.11

4D-hydroxysphinganine for IV, formerly

known as phytosphingosine;

(4E)-sphingenine for sphingosine (V);

(4Z)-sphingenine for the geometric isomer of sphingosine (VI);

D-threo-2-amino-1,3-octadecanediol for the C-2 epimer of sphinganine (II); cf. Lip. 1.10, Ex. 1.

3. Glycerol derivatives

Lip 1.12 Esters, ethers and other O-derivatives of glycerol are designated according to Carb-15 of the Rules of Carbohydrate Nomenclature (5), i.e. by a prefix, denoting the substituent, preceded by a locant. If the substitution is on a carbon atom, the compound is designated by its systematic name and not as a derivative of glycerol (e.g., 1,2,3-nonadecanetriol for $C_{16}H_{33}$ CHOH-CHOH-CH₂OH, which could be considered as 1-C-hexadecylglycerol). It is permissible to omit the locant "O" if the substitution is on the oxygen atoms of glycerol.

Examples:

tristearoylglycerol or tri-O-stearoylglycerol

or glycerol tristearate, or glyceryl tristearate; 1,3-benzylideneglycerol or 1,3-O-benzylideneglycerol; glycerol 2-phosphate (a permissible alternative to this term is 2-phosphoglycerol) (10).

Comment. The alternative system set forth in Carb-16 of the Rules on Carbohydrate Nomenclature (5), i.e. the use of the suffix "-ate," is less suitable for glycerol esters, with the exception of the phosphates (see *Examples*). However, this system may be used to designate esters of monofunctional alcohols, e.g. cholesteryl palmitate (cf. Lip 1.6).

Lip 1.13 Stereospecific numbering. In order to designate the configuration of glycerol derivatives, the carbon atoms of glycerol are numbered stereospecifically. The carbon atom that appears on top in that Fischer projection that shows a vertical carbon chain with the hydroxyl group at carbon-2 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, immediately preceding the glycerol term, from which it is separated by hyphen. The prefix "rac-" (for racemo) precedes the full name if the product is an equal mixture of both antipodes; the prefix "X-" may be used when the configuration of the compound is either unknown or unspecified (cf. Lip 1.10). Examples:

sn-glycerol 3-phosphate for the stereoisomer (VII=VIII), previously known as either L-α-glycerophosphate or as D-glycerol 1-phosphate;
rac-1-hexadecylglycerol;
1,2-dipalmitoyl-3-stearoyl-X-glycerol

Comments. i) The problem of distinguishing between stereoisomers was discussed in extenso in the 1967 document (1). In brief, difficulties arise because glycerol is a prochiral compound. The parent substance of many phospholipids, natural glycerol phosphate, has been named both as L- α -glycerol phosphate (7) (VII) and, according to standard rules of nomenclature, D-glycerol 1-phosphate (8) (VIII). When the R/S system (sequence rule) is applied, substitution of one of the primary hydroxyl groups often leads to changes in the configurational prefix, thus obscuring chemical and biogenetical relationships; it is generally inapplicable to the steric description of such mixtures as occur in triacylglycerols isolated from natural sources. The stereospecific numbering of glycerol and its derivatives as proposed by Hirschmann (9), described above and in (1), avoids these difficulties; it has proved useful and is widely accepted.

ii) The enantiomer of *sn*-glycerol 3-phosphate (VII) is *sn*-glycerol 1-phosphate (IX), as is evident from the structures.

 $\begin{array}{ccc} CH_2OH & CH_2OPO_3H_2 \\ \vdots & \vdots \\ HO \bullet C \bullet H & \equiv & H \bullet C \bullet OH \\ \vdots & CH_2OPO_3H_2 & CH_2OH \\ VII & \equiv & VIII \end{array}$

sn-Glycerol 3-phosphate [L-(glycerol 3-phosphate) \equiv D-(glycerol 1-phosphate)]

sn-Glycerol 1-phosphate [L-(glycerol 1-phosphate) ≡ D-(glycerol 3-phosphate)]

C. Symbols and Abbreviations

Lip. 1.14 The term "fatty acids" (cf. Lip 1.1) should not be abbreviated. The use of abbreviations like "FFA" for "free fatty acids" or "NEFA" for "nonesterified fatty acids" is strongly discouraged.

Comment. The words "acids" and "esters" serve to distinguish the "free" (nonesterified) and "bound" (esterified) fatty acids and are as short or shorter than the abbreviations themselves.

Lip 1.15 In tables and discussions where various fatty acids are involved, the notation giving the number of carbon atoms and of double bonds (separated by a colon) is acceptable, e.g. 16:0 for palmitic acid, 18:1 for oleic acid. Also, terms such as "(18:0)acyl" may be used to symbolize radicals of fatty acids. (See Appendix A).

Comment. This system is already widely used. It should, however, be kept in mind that it sometimes does not completely specify the fatty acid. For example, α -linolenic acid and

 γ -linolenic acid are both 18:3 acids; the designation 18:3 is therefore ambiguous. In such a case, the position of double bonds should be indicated, e.g. 18:3(9,12,15) for (9,12,15)-linolenic acid, formerly known as α -linolenic acid.

Lip 1.16 It is sometimes desirable (for example, in discussing the biosynthesis of lipids) to indicate the position of each double bond with reference not to the carboxyl group (always C-1), but to the end of the chain remote from the carboxyl. If n is the number of carbon atoms in the chain (i.e., the locant of the terminal methyl group) and x is the (lower) locant of the double bond, the position of the double bond may be defined as (n minus x). Thus, the common position of the double bond in oleic and nervonic acids may be given as 18-9 and 24-9, respectively. This structural regularity should not be expressed as $\omega 9$.

Lip 1.17 The system described in Lip 1.15 may also be used to denote alcohols and aldehydes related to fatty acids, provided that the nature of the residue is clearly indicated either by the appropriate name of the compound(s) (e.g. 18:1 alcohol) or in the heading of the table. The 1-ene of alk-1-en-1-yl (i.e., 1-alkenyl) compounds is not counted in this system (see Lip 2.10, comment).

Lip 1.18 For many complex lipids, a representation of the structures using symbols rather than structural formulae may be useful. Symbols proposed for various constituents are given in Appendix B (see also ref. 10), and, for glycolipids, in Lip 3.13. They are constructed in analogy to those in use for amino acids (11), nucleosides (12) and saccharides (13).

II. PHOSPHOLIPIDS

A. Generic Terms

The Rules of The Nomenclature of Organic Phosphorus Compounds (also known as D-Rules) (2) recognize, for biochemical usage, the prefix "phospho-" as an alternate to "Ophosphono-" (or "N-phosphono-"). By a similar convention (10), "-phospho-" may be used as an infix to designate the phosphodiester bridge present in such compounds as glycerophosphocholine. The use of root names like "phosphatidic acid" is retained and extended (Lip 2.3-2.4).

Lip 2.1 "**Phospholipid**" may be used for any lipid containing phosphoric acid as monoor diester. Likewise, lipids containing C-phosphono groups (e.g. compound X) may be termed "phosphonolipids."

Lip 2.2 "Glycerophospholipid" signifies any derivative of glycerophosphoric acid that con-

 $\begin{array}{c}
CH_2O-CO-R'\\
\vdots\\
R''CO-O-C-H\\
\vdots\\
CH_2O-PO(OH)-CH_2CH-CO_2H\\
X
\end{array}$

A phosphonolipid

$$CH_{2}O-CO-R'$$

$$\vdots$$

$$R''CO-O \leftarrow C \leftarrow H$$

$$CH_{2}O-PO(OH)-O-CH_{2}CH-CO_{2}H$$

$$XIIa$$

$$NH_{2}$$

Phosphatidylserine (3-sn-phosphatidylserine)

tains at least one O-acyl, or O-alkyl, or O-(1alkenyl) group attached to the glycerol residue. Generic names for other classes of phospholipids may be coined according to this scheme, e.g., sphingophospholipid, inositolphospholipid.

Comment. The old terms, "phosphatide," "phosphoglyceride," and "phosphoinositide" are no longer recommended because they do not convey the intended meaning (see also Lip 1.2).

Lip 2.3 "Phosphatidic acid" signifies a derivative of a glycerol phosphate (glycerophosphate) in which both remaining hydroxyl groups of glycerol are esterified with fatty acids. The position of the phosphate group may be emphasized by stereospecific numbering.

Comment. For the most common (3-sn) phosphatidic acid and its derivatives, the locants are often omitted. However, "phosphatidyl" without locants can lead to ambiguities. It is therefore preferable to use the proper locants, for example, 2-phosphatidic acid for compound XI, and 3-sn-phosphatidylserine for XIIa.

Lip 2.4 The common glycerophospholipids are named as derivatives of phosphatidic acid, e.g. 3-sn-phosphatidylcholine (this term is preferred to the trivial name, lecithin; the systematic name is 1,2-diacyl-sn-glycero-3-phosphocholine); 3-sn-phosphatidylserine; 1-phosphatidylinositol (see comment ii below); 1,3bis(3-sn-phosphatidyl)glycerol.

Comments. i) It is understood that, in combination with compounds like ethanolamine (properly, 2-aminoethanol) or serine, which bear both hydroxyl and amino groups, substitution by phosphorus is at the hydroxyl group of

H₂O₃P-O
$$\sim$$
C \sim H
:
H₂O₃P-O \sim C \sim H
:
CH₂O-CO-R"
XI
2-Phosphatidic acid
CH₂O-CO-R
:
HO \sim C \sim H NH₂
:
CH₂O-PO(OH)-OCH₂CH-CO₂H
XIIb

CH2O-CO-R'

A 2-lysophospholipid

the ethanolamine or serine. Substitution at any other position, or where confusion may arise, requires a locant.

ii) The phosphorylated derivatives of 1-(3-sn-phosphatidyl)inositol should be called 1-phosphatidylinositol 4-phosphate and 1-phosphatidylinositol 3,4-bisphosphate, respectively. The use of "diphosphoinositide" and "triphosphoinositide" for these is discouraged, as these names do not convey the chemical structures of the compounds and can be misleading. [Cf. also Table IV in (10).]

Lip 2.5 As an alternative, generic names may be coined according to Lip 1.13, i.e. using glycerol phosphate (glycerophosphate) as the stem. In this case, the stereospecific numbering of glycerol should be used to indicate the position of the phosphoric residue as well as the other substituents (acyl-, alkyl-, 1-alkenyl). If the nature of these substituents cannot be specified, the prefix "radyl" may be used.

Lip 2.6 Derivatives of phosphatidic acids resulting from hydrolytic removal of one of the two acyl groups may be designated by the old prefix "lyso," e.g. lysophosphatidylethanolamine for compound XIIb. A locant may be added to designate the site of (hydro)lysis, 2-lyso designating hydrolysis at position 2, leaving a free hydroxyl group at this carbon atom.

Comment. The "lyso" term originated from the fact that these compounds are hemolytic. It is here redefined to indicate a limited hydrolysis of the phosphatidyl derivative (i.e., "deacyl").

Lip 2.7 The term "**plasmalogen**" may be used as a generic term for glycerophospholipids in which the glycerol moiety bears an 1-alkenyl ether group.

CH2O-CH=CH-R' CH₂O-CH=CH-R' CH₂O-CH=CH-R' OH 1 R"CO-O ►C ◄ H $HO-P-O \sim C \prec H$ HO-C-H 0 CH2O-CO-R" CH2O-PO3H2 CH2O-PO(OH)--O-R" XIV XIII XV 3-Acyl-1-(1-alkenyl)-A plasmenic acid XVa: (R" = H): sn-glycerol 2-phosphate a lysoplasmenic acid XVb: $(R'' = CH_2CH_2NH_2)$ a lysoplasmenylethanolamine CH2O-CH2CH2R' CH2O-CO-C15H31 $R''-CO-O \succ C \neg H$ C17H35-CO-O≻C -H CH₂O-PO₃H₂ CH2O-PO(OH)-OCH2CH2NH2 XVI XVII A plasmanic acid 1-Palmitoyl-2-stearoyl-sn-glycero-3-phosphoethanolamine

Lip 2.8 The term "plasmenic acid" signifies a derivative of sn-glycero-3-phosphate in which carbon-1 bears an O-(1-alkenyl) residue, and position 2 is esterified with a fatty acid (XIII). This term can also be used to name derivatives, e.g. plasmenylethanolamine.

Comments. i) The use of "phosphatidyl" as a name for the acyl radical of phosphatidic acid has facilitated the nomenclature of its various compounds (see Lip 2.4). Therefore, it seems logical to offer a similar short term for XIII, i.e., "plasmenic acid," as an alternative to the more systematic name, 2-acyl-1-alkenyl-snglycerol 3-phosphate, which, of course, may be used if desired. "Plasmenic" is a contraction of "plasmalogenic" and may be especially useful in naming derivatives, e.g., plasmenylserine.

ii) Isomers like those bearing the phosphate residue in position 2 (e.g. compound XIV) should not be named in this way but as derivatives of the corresponding glycerophosphate, using stereospecific numbering.

Lip 2.9 The term "lysoplasmenic acid" may be used for a derivative of *sn*-glycero-3-phosphate that has an O-(1-alkenyl) residue on carbon-1, the hydroxyl group in position 2 being unsubstituted (XVa). This name may also be used in combinations like "lysoplasmenylethanolamine" (XVb).

Lip 2.10 For compounds of type XVI, bearing a saturated ether group in position 1 and an acyl group in position 2 of *sn*-glycero-3phosphate, the term "**plasmanic acid**" is proposed. Compounds deacylated in position 2, or with a substituent on the phosphoric residue, can be treated as are the plasmenic acids (Lip 2.9).

Comment. The proposed names will be especially useful for naming phosphoric diesters (phosphodiesters), e.g., plasmanylethanolamine, instead of 2-acyl-1-alkyl-sn-glycero-3-phosphoethanolamine. The terms "plasmanic acid" and "plasmanyl" may also be applied to ethers with an alkyl group bearing a double bond within the chain, e.g. a 9-hexadecenyl residue (derived from palmitoleic acid). In such cases, the proper term "alkenyl," if used without the ene locant(s), would be misleading. (See Lip 1.17).

B. Individual compounds

Lip 2.11 Individual glycerophospholipids in which the substituents can be specified are named according to existing Rules (2,3,5,6), using the infix "-phospho-" (2,10) to indicate the phosphodiester bridge.

Example:

1-Palmitoyl-2-stearoyl-sn-glycero-

3-phosphoethanolamine for compound XVII.

Lip 2.12 The ketone derived from glycerol, 1,3-dihydroxy-2-propanone, also known as dihydroxyacetone, may be termed "glycerone," if desired. The name is a contraction of "glyceroketone" and may be useful to emphasize the relationship with glycerol, glyceraldehyde (glyceral), and glycerate. It also permits a simple symbolism (Appendix B) and the naming of derived lipids, e.g., 1-palmitoyl-3-phosphoglycerone.

III. GLYCOLIPIDS

A. General Considerations

Glycolipids (a contraction of glycosyllipids) are generally named as glycosyl derivatives of the corresponding lipid, e.g., diacylgalactosyl-glycerol, glucosylceramide. Because of the heterogeneity of the fatty acids and long-chain bases encountered in most cases, a generic name for the lipid moiety is needed, i.e. ceramide. With higher glycosphingolipids, especially the gangliosides, naming problems arise from the complexity of the carbohydrate moiety of these compounds. The systematic names of the oligosaccharides linked to ceramide are so cumbersome that they are of the same practical value as, e.g., the systematic name for a peptide hormone such as insulin. It was felt that this difficulty could be overcome only by creating suitable trivial names for some parent oligosaccharides. In constructing these names (see Table I) the following principles were observed:

1. The number of monosaccharide units in an oligosaccharide is indicated by the suffixes "-biose," "-triaose," "-tetraose," etc. This follows the well-established practice in the carbohydrate field (cf. cellobiose, cellotetraose, maltotetraose, etc.), with the exception that the suffix "-triose," as used in maltotriose, has been changed to "-triaose" to avoid confusion with the monosaccharides called trioses.

2. The oligosaccharides are grouped in series according to their structure and biogenetic relationship.

3. Differences in linkage (e.g., $1 \rightarrow 4$ versus $1 \rightarrow 3$) in otherwise identical sequences are indicated by "iso-" or "neo-," used as a prefix. On the basis of these names, the semisystematic nomenclature for neutral glycosphingolipids and gangliosides described below is recommended. A set of symbols has been devised that allows a simple representation of complex neutral and acidic glycosphingolipids (Table I).

B. Generic Terms

Lip 3.1 The term "glycolipid" designates any compound containing one or more monosaccharide residues linked by a glycosyl linkage to a lipid part [e.g., a mono- or diacylglycerol, a long-chain base (sphingoid) like sphingosine, or a ceramide].

Lip 3.2 The term "glycoglycerolipid" may be used to designate glycolipids containing one or more glycerol residues.

Lip 3.3 The term "glycosphingolipid," as hitherto, includes all compounds containing at least one monosaccharide and a sphingoid. The glycosphingolipids can be subdivided as follows:

Neutral glycosphingolipids:

Monoglycosyl- and oligoglycosylsphingoids; monoglycosyl- and oligoglycosylceramides. Acidic glycosphingolipids:

sialosylglycosylsphingolipids (gangliosides); sulfoglycosylsphingolipids (formerly

"sulfatides," which is not recommended) (cf. Lip 3.11).

Lip 3.4 "Psychosine" may be used as a generic name for 1-monoglycosylsphingoids, although the latter is preferred. The nature of the monosaccharide and the sphingoid is not specified in this name.

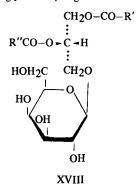
Lip 3.5 The term "fucolipid" may be used to designate fucose-containing neutral or acid glycolipids.

C. Individual Compounds*

Lip 3.6 Glycoglycerolipids may be named either as glycosyl compounds according to Rule Carb-24 or as glycosides according to Rule Carb-23 (5).

Example:

Compound XVIII may be named either 1,2-diacyl-3- β -D-galactosyl-sn-glycerol or 1,2-diacyl-sn-glycerol 3- β -D-galactoside.



Comment. The first form is preferred, as the glycosphingolipids are also named this way.

Lip 3.7 A glycosphingolipid is generally named as a "glycosylsphingoid" or a "glycosylceramide," using the appropriate trivial name of the mono- or oligosaccharide residue for "glycosyl." It is understood that the sugar residue is attached to the C-1 hydroxyl group of the ceramide. For glycosphingolipids carrying two to four saccharide residues, the trivial names listed in Table I are recommended.

*"Individual" in this section refers to the carbohydrate moiety only. *Comment.* It is strongly recommended that the name of the oligosaccharide be defined in each publication by means of the standard symbols for sugars (as in Table I, column 1) rather than by the full name, which is often so long as to be confusing.

Lip 3.8 The trivial name "cerebroside" designates $1-\beta$ -glycosylceramide (the natures of the sphingoid and of the fatty acid are not specified in this name).

Lip 3.9 Glycosphingolipids carrying fucose either as a branch or at the end of an oligohexosylceramide are named as "fucosyl(X)osylceramide" where (X) stands for the root name of the oligosaccharide. The location of the fucosyl residue is indicated by a Roman numeral designating the position of the monosaccharide residue in the parent oligosaccharide (counting from the ceramide end) to which the fucose residue is attached, with an Arabic numeral superscript indicating the position within that residue to which the fucose is attached. If necessary, the anomeric symbol can be used as usual, i.e., preceding "fucosyl-."

Examples for Lip 3.7 and Lip 3.9 (structures given in the symbols of Lip 3.13):**

Lactosylceramide for Gal $(\beta 1 \rightarrow 4)$ GlcCer; mucotriaosylceramide for

Gal(β 1 \rightarrow 4)Gal(β 1 \rightarrow 4)GlcCer;

III²-α-fucosylisoglobotriaosylceramide for

 $\operatorname{Fuc}(\alpha 1 \rightarrow 2)\operatorname{Gal}(\alpha 1 \rightarrow 3)\operatorname{Gal}(\beta 1 \rightarrow 4)\operatorname{Glc}(\beta 1 \rightarrow 1)\operatorname{Cer}.$

Lip 3.10 Sialoglycosphingolipids (synonym: gangliosides) are glycosphingolipids carrying one or more sialic residues. Sialic acid is the generic term for N-acetyl- or N-glycoloylneur-aminic acid (cf. section 3 in ref. 1). Ganglio-sides are named as N-acetyl- (or N-glycoloyl-) neuraminosyl-(X)osylceramide, where (X) stands for the root name of the neutral oligo-saccharide to which the sialosyl residue is attached (cf. Table I). The position of the sialosyl residue is indicated in the same way as in the case of fucolipids (see Lip 3.9).

Example:

II³-N-acetylneuraminosyllactosylceramide for AcNeu($\alpha 2 \rightarrow 3$)Gal($\beta 1 \rightarrow 4$)Glc($\beta 1 \rightarrow 1$)Cer

Lip 3.11 Glycosphingolipids carrying a sulfuric ester (sulfate) group, formerly called sulfatides, are preferably named as sulfates of the parent neutral glycosphingolipid. The location of the sulfate group may be indicated as in Lip. 3.9.

Example:

lactosylceramide II³-sulfate

Lip 3.12 Phosphoglycosphingolipids with phosphodiester structures are named according to the recommendation for the phospholipids (see Section II).

D. Symbols and Abbreviations.

Lip 3.13 Simple or complex glycosphingolipids can be represented according to existing rules, using the symbols Cer, Sph, AcNeu, etc. (Appendix B), together with the recommended (13) symbols for the hexoses (Glc, Gal, etc.). Examples are given above, and in Table I and Appendix C. However, due to the complexity of the higher glycosphingolipids, this often results in very long and cumbersome series that are not easy to comprehend. It is therefore recommended that the oligosaccharides listed in Table I be represented by specific symbols in which the number of monosaccharide units (-oses) is indicated by Ose_n , preceded by two letters representing the trivial name of the oligosaccharide (column 3). For a short form, which may be required in the case of limited space or frequent repetition, Ose can be omitted (column 4); however, the long form is preferred as being more evocative.

Examples:

- (i) McOse₃Cer for mucotriaosylceramide, Gal(β1-4)Gal(β1-4)Glc(1-1)Cer;
- (ii) II³AcNeu-GgOse₄Cer for II³-Nacetylneuraminosylgangliotetraosylceramide, Galβ1→3GalNAcβ1→4Gal(3←2αNeuAc)β1→ 4Glcβ1→1Cer (see Lip 3.14 for this mode of representing a branched chain.).

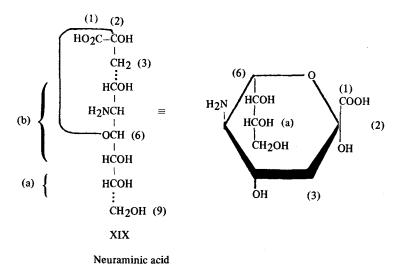
Abbreviations for the more important gangliosides are given in Appendix C.

Lip 3.14 When it is desirable to represent a branched oligosaccharide on a single line, as in running text or a table, the parentheses surrounding the locants in the main chain may be omitted and used instead to enclose the symbols for the branched portion(s) of the molecule. The branches follow, in parentheses and with appropriate arrows, the residues to which they are attached.

Examples:

- (i) NeuGc $\alpha 2 \rightarrow 3$ Gal $\beta 1 \rightarrow 3$ GalNAc $\beta 1 \rightarrow 4$ Gal $(3 \leftarrow 2\alpha$ NeuGc $)\beta 1 \rightarrow 4$ Glc $\beta 1 \rightarrow 1$ Cer;
- (ii) NeuAc α 2 \rightarrow 3Gal β 1 \rightarrow 3GalNAc β 1 \rightarrow 4Gal(3 \leftarrow 2aNeuAc β \leftarrow 2aNeuAc β
- $4Gal(3\leftarrow 2\alpha NeuAc8\leftarrow 2\alpha NeuAc)\beta1\rightarrow 4Glc\beta1\rightarrow 1Cer$ (iii) GalNAc α 1 \rightarrow 3Gal(2 \leftarrow 1 α Fuc) β 1 \rightarrow
 - 4GlcNAc($3 \leftarrow 1 \alpha$ Fuc) $\beta 1 \rightarrow 3$ Gal $\beta 1 \rightarrow 4$ Glc $\beta 1 \rightarrow 1$ Cer
 - \equiv III³,IV²- α , α -Difucosyl-IV³- α -2-acetamido-
 - $\label{eq:loss_loss} 2 \text{-} deoxy galactosyl neolactote traosyl ceramide}$
 - $\equiv III^{3}IV^{2}(Fuc\alpha)_{2}, IV^{3}GalNAc\alpha nLcOse_{4}Cer.$

^{**}D is omitted by convention in the abbreviated formulas, but D (or L) may be inserted when desirable. Hyphens may replace left-to-right arrows (see section 3.4 of ref. 13).



5-Amino-3,5-dideoxy-D-glycero-D-galacto-nonulopyranosonic acid

(a) (b)

IV. NEURAMINIC ACID

Lip 4.1 The compound 5-amino-3,5-dideoxy-D-glycero-D-galacto-nonulosonic acid is neuraminic acid (XIX), with the symbol Neu (11).

Lip 4.2 The term "sialic acid" signifies the N-acylneuraminic acids and their esters and other derivatives of the alcoholic hydroxyl groups.

Lip. 4.3 The radicals resulting from the removal of a hydroxyl group of neuraminic acid or sialic acid are designated as **neuraminoyl** or **sialoyl**, respectively, if the hydroxyl is removed from the carboxyl group, and as **neuraminosyl** and **sialosyl**, respectively, if the hydroxyl group is removed from the anomeric carbon atom of the cyclic structure.

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	Names and Abbreviations of Simple Glycolipids		
Structure ^a	Trivial name of Oligosaccharide ^b	Symbolc	Short symbold
Gal(α 1-4)Gal(β 1-4	Globotriaose Globotetraose Isoglobotriaose	GbOse3 GbOse4 iGbOse3	Gb3 Gb4 Gb4 iGb3
Gair/Arc(p1-2)Gair(q1-3)Gair(p1-4)GicCer Gair(g1-3)Gair(g1-4)Gair(g1-4)GicCer Gair(g1-3)Gair(g1-4)Gair(g1-4)GicCer	isogiopotetraose Mucotriaose Mucotetraose	1GDUse4 McOse3 McOse4	1Gb4 Mc3 Mc4
GlcN Ac(81-3)Gal(81-4)GtcCer Gal(81-3)GlcN Ac(81-3)Gal(81-4)GlcCer Gal(81-4)GlcN Ac(81-3)Gal(81-4)GlcCer	Lactotriaose Lactotetraose Neolactotetraose	LcOse3 LcOse4 nLcOse4	Lc3 Lc4 nLc
Gal(eta_1 -3)Gal(eta_1 -4)Gal($$	Gangliotriaose Gangliotetraose	GgOse3 GgOse4	Gg3 Gg4
Gal(α1-4)GalCer Gal(1-4)Gal(α1-4)GalCer GalNAc(1-3)Gal(α1-4)GalCer	Galabiose Galatriaose N-Acetylgalactosaminylgalatriaose	GaOse2 GaOse3 GaINAc1-3GaOse3	Ga2 Ga3
^a Symbols and arrangement are discussed in Lip 3. ^b Name of glycolipid is formed by converting endi ^c Should be followed by Cer for the glycolipid, wi ^d The short form should be used only in situation.	^a Symbols and arrangement are discussed in Lip 3.13. Hyphens replace left-to-right arrows (see Section 3.4 of ref. 13). ^b Name of glycolipid is formed by converting ending "-ose" to "-osyl," followed by "-ceramide," without space; e.g., globotriaosylceramide. ^c Should be followed by Cer for the glycolipid, without space; e.g., McOse3Cer, Mc4Cer (see Lip 3.13). ^d The short form should be used only in situations of limited space or in case of frequent repetition.	of ref. 13). Þace; e.g., globotriaosylceramide.	

TABLE I

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	Numerical	Structure	Sten	Stems of	"omeN"
	Symbol	$H_3C-(R)-CO_2H$	Systematic Names ^a	Trivial Names ^b	Symbol
Ŧ	10:0	-(CH ₂) ₈ -	Decano-	Capr-c	Dec
6	12:0	-(CH3)10-	Dodecano-	Laur-	Tau
ŝ	14:0	-(CH2)13-	Tetradecano-	Mvrist-	Mvr
4	16:0	-(CH2)12-	Hexadecano-	Palmit-	Dem
ŝ		-(CH2) CH=CH(CH2)	9-Hexadeceno-	Palmitole-	APam
9		-(CH ₂)1 2	Octadecano-	Stear-	
٢	18:1(9)	$-(CH_3)_7CH=CH(CH_3)_7-$	cis-9-Octadeceno-	Ole-	90
8	18:1(11)	-(CH ₂), CH=CH(CH ₂),	11-Octadeceno-	Vaccen-	Var
6		-(CH5)3(CH2CH=CH)3(CH2)7-	cis.cis-9.12-Octadecadieno-	Linole-	l in
10	18:3(9,12,15)	-(CH ⁵ CH=CH) ₃ (CH ₃) ⁷ -	9.12.15-Octadecatrieno-	(9.12.15)-Linolen-	nu. Iv
11	~	-(CH2)3(CH5CH=CH)3(CH2)2-	6,9,12-Octadecatrieno-	(6.9.12)-Linolen-	uu lv
12	18:3(9,11,13)	-(CH ₂) ₃ (CH=CH) ₃ (CH ₂) ₇ .	9,11,13-Octadecatrieno-	Eleostear-	eSte
13		-(CH ₂)18-	Icosanod	Arachid-	Ach
14	20:2(8,11)	-(CH3), (CH3 CH=CH), (CH3), -	8.11-tcosadieno-d		Ac Ach
15	[1]	-(CH2), (CH2CH=CH) 2(CH2) 2-	5.8.11-Icosatrieno-d		
16	20:4(5,8,11,14)	-(CH ₃) ₃ (CH ₃ CH=CH) ₄ (CH ₃) ₃ -	5,8,11,14-Icosatetraeno-d	Arachidon-	
17	22:0	-(CH3)30-	Docosano-	Behen-	Beh
18	24:0	-(CH2)22-	Tetracosano-	Lignocer-	Lie
19	24:1	-(CH ₂)7CH=CH(CH ₂)13-	cis-15-Tetracoseno-	Nervon-	Ner
20	26:0	-(CH3),4-	Hexacosano-	Cerot-	t-C
21	28:0	$-(CH_2)_{26}^{-}$	Octacosano-	Montan-	Mon
	¹ Ending in ''-ic" acid, '- _'	^{a Ending} in "-ic" acid, "-ate," "-yl", for acid, salt or ester, acyl radical, respectively.	l, respectively.		

^cNot recommended because of confusion with caproic (hexanoic) and caprylic (octanoic) acids. Decanoic is preferred.

^bEnding in "-ic acid," "-ate," "-oy1" for acid, salt or ester, or acyl radical, respectively.

dFormerly "eicosa-" (Changed by IUPAC Commission on Nomenclature of Organic Chemistry, 1975.)

Names of and Symbols for Higher Fatty Acids

APPENDIX A

NOMENCLATURE OF LIPIDS

LIPIDS, VOL. 12, NO. 6

APPENDIX B

Symbols Recommended for Various Constituents of Lipids

Name	Symbol ^a
For alkyl radicals ^b	R
Methyl, Ethyl, Dodecyl	Me, Et, Pr, Bu, Pe, Hx, Hp, Oc, Nn, Dec, Und, Dod
For aliphatic carboxylic acids ^b	acyl (not abbreviated), RCO-
Formyl, Acetyl, Glycoloyl, Propionyl,	Fo (or HCO), Ac, Gc, Pp,
Butyryl, Valeryl,	Bt, VI,
Hexanoyl, Heptanoyl, Octanoyl,	Hxo, Hpo, Oco,
Nonanoyl, Decanoyl, Undecanoyl,	Nno, Dco, Udo,
Lauroyl, Myristoyl, Palmitoyl,	Lau, Myr, Pam,
Stearoyl, Eleostearoyl, Linoleoyl, Arachidonoyl	Ste, eSte, Lin, A4Ach
For glycerol and its oxidation products ^c	
Glycerol, Glyceraldehyde, Glycerone, Glyceric acid	Gro, Gra, Grn, Gri.
For "glycosyl"	Ose
Glucose, Galactose, Fucose,	Glc ^d , Gal, Fuc
Gluconic acid, Glucuronic acid •	GlcA, GlcU ^e
Glucosamine ^f , N-Acetylglucosamine	GlcN, GlcNAc
Neuraminic, Sialic, Muramic acids	Neu, Sia, Mur
N-Acetylneuraminic acid, N-Glycoloylneuraminic acid	NeuAc ^g , NeuGc
Deoxy	d
Miscellaneous	
Ceramide, Choline, Ethanolamine,	Cer, Cho, Etn ^h ,
Inositol, Serine,	Ins, Ser,
Phosphatidyl, Sphingosine, Sphingoid, Phosphoric	- ,
residue.	Ptd, Sph, Spd, P.

^aThese symbols are constructed in analogy to those already in use for amino acids and saccharides (11,13); they may assist the abbreviated representation of more complex lipids in a way similar to the peptides and polysaccharides. Prefixes such as "iso-," "tert-," "cyclo-" are specified in the symbols by lower-case superscripts (Prⁱ, Bu^t, Hx^c) or lower-case prefixes (iPr, tBu, cHx), unsaturation by, e.g., Δ^3 for a 3,4 double bond, Δ^3 for a 3,4 triple bond (cf. Proteins, Vol. I, pp. 96-108, in *Handbook of Biochemistry*, 3rd edition, edited by G. Fasman, CRC Press, Cleveland, OH, 1976). Many of these symbols are drawn from previously published Recommendations (refs. 11,12). See also Appendix A.

^bSystematic and recommended trivial names of unbranched, acyclic compounds only (cf. Appendix A). Other forms are created by prefixes (e.g., "iso-," "tert-," "cyclo-"). See Appendix A.

^CThese symbols form a self-consistent series for a group of closely related compounds. It is recognized that other abbreviations (but no symbols) are currently in use. (See Lip 2.12.)

^dNot Glu (glutamic acid) or G (nonspecific).

^eRecommended in place of GlcUA, the "A" being unnecessary.

 $^{\rm f}$ Approved trivial name for 2-amino-2-deoxyglucose; similarly for galactose (GalNAc), etc.

gAcNeu was recommended earlier (ref. 11). When it is necessary to differentiate between N-acetyl and O-acetyl derivatives, NeuNAc and NeuOAc (italicized locants, in contradistinction to GalNAc, etc.) may be employed.

^hMay take the form OEtN < if substitution on the nitrogen atom is to be indicated.

NOMENCLATURE OF LIPIDS

APPENDIX C

Abbreviated Representation of Gangliosides

	Lipid Document ^a	Designation according to Wiegandt ^b	Svennerholm ^c
1.	1 ³ NeuAc-GalCer	G _{Gal} 1 NeuAc	
2.	II ³ NeuAc-LacCer	G _{Lac} 1 NeuAc	G _{M3}
3.	II ³ NeuGc-LacCer	G _{Lac} 1 NeuNGI	_
4.	II ³ (NeuAc) ₂ -LacCer	G _{Lac} 2 NeuAc	GD3
5.	II ³ NeuAc/NeuGc-LacCer	G _{Lac} 2 NeuAc/NeuNG	
6.	II ³ NeuGc-LacCer	G _{Lac} 2 NeuNGl	_
7.	II ³ NeuAc-GgOse ₃ Cer	G _{Gtri} 1 NeuAc	G _{M2}
8.	II ³ NeuAc-GgOse ₄ Cer	GGtet 1 NeuAc	G _{M1}
9.	IV ³ NeuAc-nLcOse ₄ Cer	GLntet 1a NeuAc	GM1-GlcNAc
10.	IV ⁶ NeuAc-nLcOse ₄ Cer	GLntet 1b NeuAc	_
11.	IV ² Fuc,II ³ NeuAc-GgOse ₄ Cer	G _{Gfpt} 1 NeuAc	
12.	IV ³ NeuAc-nLcOse ₄ Cer		_
13.	II ³ (NeuAc) ₂ -GgOse ₄ Cer	G _{Gtet} 2b NeuAc	GD1b
14.	IV ³ NeuAc,II ³ NeuAc-GgOse ₄ Cer	G _{Gtet} 2a NeuAc	GD1a
15.	II ³ (NeuAc) ₃ -GgOse ₄ Cer	GGtet 3b NeuAc	-
16.	IV ³ NeuAc,II ³ (NeuAc) ₂ -GgOse ₄ Cer	G _{Gtet} 3a NeuAc	G _{T1}
17.	IV ³ NeuAc.II ³ (NeuAc) ₂ -GgOse ₄ Cer	GGtet 4b NeuAc	_
18.	IV ³ (NeuAc) ₂ II ³ (NeuÁc) ₃ -GgOse ₄ Cer	GGtet 5 NeuAc	-
19.	IV ³ NeuAc,II ³ NeuAc-GgOse ₅ Cer	G _{Gpt} 2a NeuAc	_

^aTo indicate linkage points and anomeric form: Fuc should be written ($\leftarrow 1\alpha$ Fuc); NeuAc should be written ($\leftarrow 2\alpha$ NeuAc); (NeuAc)₂ should be written ($\leftarrow 2\alpha$ NeuAc8)₂; etc. If these features are assumed or defined, the short form used in this column is more convenient for use in texts and tables.

^bThe subscripts to G (for ganglioside), from 7 on, have the meanings: Gtri =gangliotriose, Gtet = ganglio-tetraose, Litet = lactoisotetraose, Gpt = gangliopentaose, Gfpt = gangliofucopentaose [Ref. H. Wiegand, Hoppe-Seyler's Z. Physiol. Chem. 354:1049 (1973)]. ^cG = ganglioside, M = monosialo, D = disialo, T = trisialo. Arabic numerals indicate sequence of migration in thin-layer chromatograms [Ref. Svennerholm, L., J. Neurochem. 10:613 (1963)].