Segment Nomenclature of Organic Compounds†

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Received February 22, 1995⊗

In the proposed system for naming organic compounds, the structure to be named is divided into homogeneous segments made of ring systems, heteroatoms, or acyclic carbon chains which, together with their substituents, are then numbered and named, independently of each other, by current organic nomenclature. The set of names of segments makes the segment name of the structure. To select the direction of citation in segment names, seniority rules for all the types of segments are used. The segment nomenclature obviates selection of parent structure and principal group, ambiguous numbering of acyclic carbon chains, and use of a hierarchy of enclosing marks. The segment nomenclature generates unique names which are simpler and more comprehensible than current names, especially for complex structures containing besides acyclic carbon chains several ring systems and/or heteroatoms. Both construction of the name from a structure and deducing the structure from a name are comparatively easy. The segment nomenclature is not intended for general use; however, it may be suited for implementation in computer software.

INTRODUCTION

Traditionally, organic nomenclature has been substitutive, i.e., based on a central unit, parent system, in the structure to which all other units are substituents. Out of the substituents, current organic nomenclature, using special seniority rules, selects one which is then cited as a suffix, the other being expressed as prefixes.[1,2] The substitutive nomenclature works well for both cyclic and acyclic compounds. However, interruption of an acyclic carbon chain at several sites by rings and/or heteroatoms brings about complications as it is necessary to treat these structure units as additional centers. For more complex structures, the centric approach in the naming inevitably leads to intricate and cumbersome names. A striking example is the following name[3] for a comparatively simple compound using the hierarchy of six enclosing marks: 4,4′-{1-[({5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy)carbonyl]ethylene}-dibenzoic acid (see Appendix 2, example 13).

Such names are hardly comprehensible and both construction of the name from the structure and writing the structure on the basis of the name require much effort and attention to avoid errors. For structures containing several discontinuities, substitutive nomenclature seems to fail and, consequently, the need for noncentric, "continuous" nomenclature arises. Generally, development of a new systematic organic nomenclature, which would be more computer-friendly than current nomenclature systems on one hand and more readily understandable for manual users on the other, is highly desirable.[4]

In an effort to find an alternative system of naming organic compounds, the author was inspired by the naming of constitutional repeating units in regular single-strand organic polymers.[5] (A similar method was proposed for naming macrocycles.[6]) The new system proposed for naming organic compounds is not centric: it does not name a compound as a whole. Instead, it divides the structure into several segments and the set of the names of segments makes then the name of a compound. To be easily named, the segments are selected in such a way that they are made of ring systems, heteroatoms, or acyclic carbon chains. As the nomenclature of the three classes of compounds is elaborated in great detail, naming the respective segment types does not make major difficulties.

PRINCIPLES OF SEGMENT NOMENCLATURE

For an easier understanding of the procedure proposed, a list of the terms and concepts used and their definitions are given here.

Ring System. A single ring, fused rings, spiro systems, polycyclic bridged systems, or ring assemblies (rings of the same type linked together).

Heteroatom System. A single heteroatom or heteroatom array (heteroatoms of the same type linked together).

Segment. A heterocyclic ring system, carbocyclic ring system, heteroatom system, or acyclic carbon chain (not including substituents to them).

Chain. A part of structure consisting of one or more segments arranged linearly. In most cases, the chain contains two terminal segments of connectivity 1 and *n* inner segments of connectivity 2 where $n = 0,1,2,...$

Chain Length. The number of segments in the chain.

Acyclic Carbon Chain Length. The number of carbon atoms in the chain (not including substituents).

Heteroatom Array Length. The number of heteroatoms in the array (not including substituents).

Seniority of Segments. The basic order of seniority is as follows: heterocyclic ring system > heteroatom system > carbocyclic ring system > acyclic carbon chain. For a detailed order of seniority of segments, see Appendix 1.

To construct the name of a structure using the segment nomenclature, the following steps are to be done in order: identification of segments in chains, identification of the main chain, orientation of the main chain, numbering of segments,

† Presented in part as a poster communication at Commemorative Symposium on the Centennial Anniversary of the "Geneva Conference", Geneva, April 22−24, 1992.

⊗ Abstract published in *Advance ACS Abstracts,* November 1, 1995.

0095-2338/96/1636-0001$12.00/0

naming of segments, naming of the structure. The instructions and notes corresponding to the steps given are as follows.

Identification of Segments in Chains. All chains in the structure are divided into segments.

Identification of the Main Chain. Main chain is the longest chain in the structure. (Considering a chain all other branches are taken as substituents to it.) If two or more chains are of the same maximum length, the main chain is selected using the following criteria until a decision is reached:

−highest total length of acyclic carbon chains and heteroatom arrays in the chain;

−highest seniority of both terminal segments in the chain;

−highest seniority of both penultimate segments in the chain;

−highest seniority of both segments before penultimate segments in the chain.

Orientation of the Main Chain. The main chain is oriented in such a way that the terminal segment of higher seniority is on the left, that of lower seniority on the right. If both the terminal segments are of the same seniority, the penultimate segments are compared, etc. until a decision is reached.

Numbering of Segments. Each segment is numbered independently of the others.

Ring segments are numbered in accord with their fixed numbering. If there is a choice in the nonterminal segments, the free valence atom on the left side of the main chain segment or on the side nearer to the structure periphery in the side chain segment has the lowest possible locant. If there is a choice in the terminal segment, the free valence atom has the lowest possible locant.

Heteroatom Array and Acyclic Carbon Chain Segments. In nonterminal segments, the atom on the left side of the main chain segment or on the side nearer to the structure periphery in the side chain segment bears locant 1. In terminal segments, the free valence atom has locant 1.

Note. Alternatively, in acyclic carbon chains (see naming of segments, note 2), the atoms mentioned above may bear the lowest possible locants instead of locant 1.

Naming of Segments. Generally, terminal segments are named as monocoordinate, mono-, or higher-valent units, whereas nonterminal segments are named as double-coordinate, di-, or higher-valent units, according to the rules of nomenclature of organic chemistry.[1,2]

For naming purposes, terminal segment together with the next segment make one merged terminal segment, which is named as a whole by the terminal-type name. (This is in particular the case of common terminal two-segment groups like SO_2OH, COOH, NO_2, NHOH, CHO, and CN, which are regarded as one segment.) The name of segment includes as prefixes the names of substituents and side chains bonded to the segment, if any, arranged alphabetically.

Note 1. Merging of terminal segments shortens the names of structures but is not necessary.

Note 2. Alternatively, the names of acyclic carbon chain segments with terminal acyclic carbon chain substituents may be based on the longest carbon chain including the substituents.

Naming of the Structure. The complete names of main chain segments (including the names and locants of side chains and substituents) are cited in order from left to right as they appear in the oriented main chain. Three-segment main chain is named using the name of the left merged terminal segment. Four- and higher-segment main chain is named using both merged terminal segment names.

The complete names of side chain segments are cited in order starting from the periphery. Two- and higher-segment side chains are named using the merged terminal segment name and nonterminal segment name(s), if needed.

The names of segments are separated by dashes.

DISCUSSION AND CONCLUSION

For the segment nomenclature, a seniority system for all the types of segments, i.e., ring systems, both heterocyclic and carbocyclic, heteroatom systems, and acyclic carbon chains, is of primary importance. At that, it is necessary to distinguish between the seniority within the same type of segments (e.g., pyridine vs oxazole) and seniority within the same segments (e.g., variously substituted pyridines or butyls).

First-type seniority for rings is treated in the Blue Book,[1] in connection with fusion nomenclature. This is also the case with the seniority among heteroatoms[1,2] which was established for the purpose of replacement nomenclature of heterocycles (Hantzsch-Widman system). Seniority of acyclic carbon chains is straightforward: it is determined by the length of the carbon chain, i.e., by the number of carbon atoms in the chain. A similar principle applies to heteroatom arrays.

So far, the second-type seniority has been treated only scantily.[1,5] It can be, however, established adequately, in accord with the modularity concept, for all the types of segments on the basis of substituents and multiple bonds in acyclic carbon chains and heteroatom arrays. The proposed general criteria are based on the number of substituents (multiple bonds), their locants, and their position in alphabet (as a last resort). Roughly speaking, the otherwise same segment containing a larger number of substituents (multiple bonds), substituents (multiple bonds) with lower locants, or substituents earlier in alphabet is senior to the other.

For detailed rules of seniority for various types of segments, see Appendix 1.

The segment nomenclature of organic compounds has several advantages over the current substitutive nomenclature. The segment nomenclature obviates the following:

−the selection of parent structure;

−searching among substituents for a principal group to be named by suffix; hence, an inevitably complicated seniority order of a large number of substituent types is unnecessary;

−the often ambiguous numbering of acyclic carbon chains which depends on the position of substituents; in contrast, the numbering in the segment nomenclature is entirely independent of the type and position of substituents;

−use of a hierarchy of enclosing marks (parentheses, square brackets, braces, etc.), common in complex substitutive names, which are difficult both to construct and to decipher and which lead to errors.

The segment nomenclature enables specific and unambiguous localization of various structural features and modifications, such as stereochemistry and isotopic modification, due to the separate and independent treatment of segments.

Chart 1

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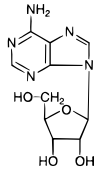

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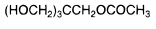

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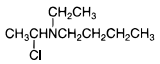

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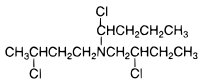

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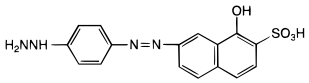

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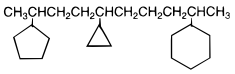

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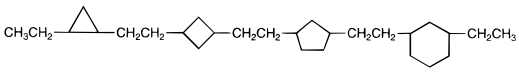

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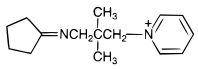

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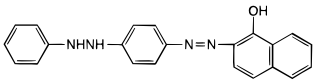

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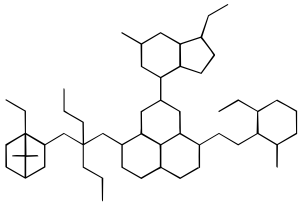

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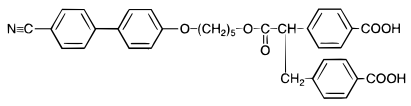

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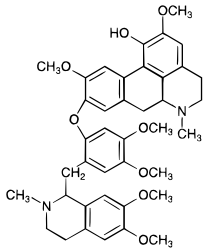

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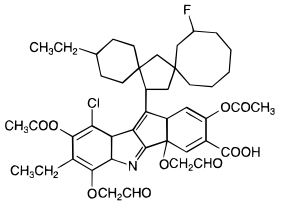

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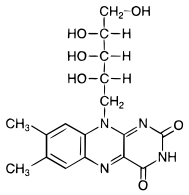

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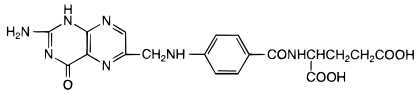

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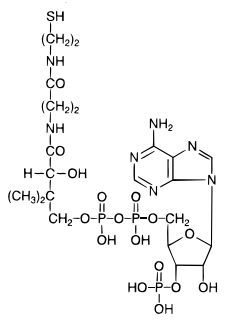

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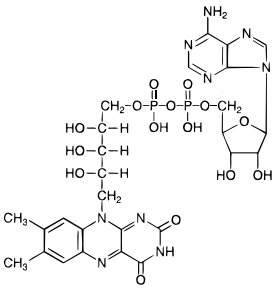

Chart 1 (continued)

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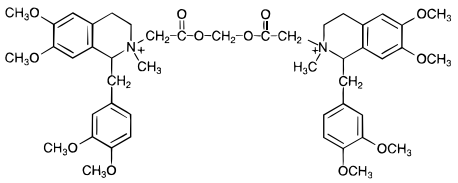

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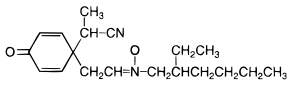

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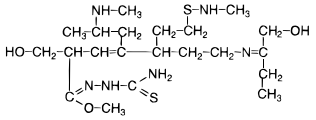

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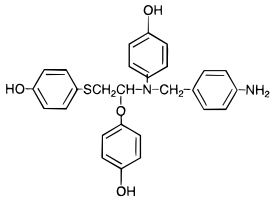

The rules for construction of segment names are easily understood and applied. Quite often, the names are simpler and more comprehensible than current names, which makes easier both construction of the name for an organic structure and deducing the structure from a name. This is especially so with structures containing rings, heteroatoms, and carbon chains.

The segment nomenclature leads to unique names in the sense that the structure has only one name and, the other way round, one name corresponds to single structure (one-to-one correspondence). Implementation of the segment nomenclature into computer software should not cause major difficulties. Using the new system, computerization of tasks such as generation of a name from chemical structure, generation of a structure from a name, searching of databases, search for partial structures, or others might be simpler. (For recent attempts at translation of structures into IUPAC names and vice versa, see refs 7 and 8.) Last but not least: unlike some other nomenclature systems,[9,10] the segment nomenclature uses the same vocabulary and terminology as current substitutive nomenclature.

The segment nomenclature is not intended for general use, nor should it displace or replace current substitutive names of organic compounds. It might be useful for special purposes, such as for complex structures, for computerization of organic structure databases, for computerized translation of names into structures and vice versa, for retrieving structure fragments, and whenever unique names for structures are necessary or, at least, more advantageous.

Examples of compounds named by currently used nomenclatures (IUPAC, Chemical Abstracts, or nonsystematic names) and by the segment nomenclature are given in Appendix 2.

APPENDIX 1. SENIORITY OF SEGMENTS

Heterocyclic Ring Systems. Among heterocyclic ring systems, the descending order of seniority is as follows:

(a) a ring system with nitrogen in the ring;

(b) a ring system containing a heteroatom other than nitrogen as high as possible in the order of heteroatoms given below;

(c) a ring system containing the greatest number of rings;

(d) a ring system having the largest individual ring;

(e) a ring system having the largest number of heteroatoms;

(f) a ring system containing the greatest variety of heteroatoms;

(g) the ring system having the greatest number of heteroatoms highest in the order given below;

(h) of the two ring systems of the same size containing the same number and kind of heteroatoms the senior ring system is that one with the lower locants for the heteroatoms.

The order of decreasing seniority within a given heterocyclic ring system is the following:

(a) when two heterocyclic systems differ only in degree of unsaturation, the senior system is that with the lowest state of hydrogenation;

(b) when two heterocyclic systems of the same degree of unsaturation differ in the positions of multiple bonds, the senior system is that having multiple bonds with the lowest locants;

(c) a ring system with the lowest locants of free valences;

(d) in assemblies of identical heterocyclic systems, the assembly of highest seniority is that having lowest numbers for the points of attachment between the systems within the assembly consistent with the fixed numbering of the systems;

(e) a ring system with the largest number of substituents;

(f) a ring system having substituents with the lowest locants;

(g) a ring system in which the substituent first in alphabetical order has the lowest locant.

Heteroatom Systems. For the most common heteroatoms the descending order of seniority is as follows:

F > Cl > Br > I > O > S > Se > N > P > As > Si > B

Other heteroatoms may be placed within this order as indicated in ref 11.

A longer heteroatom array is senior to a shorter one, i.e., a heteroatom array is senior to a single heteroatom of the same type.

The order of decreasing seniority for heteroatom arrays of equal length is:

(a) when two arrays differ only in degree of unsaturation, the senior array is that with the lowest state of hydrogenation;

(b) when two arrays of the same degree of unsaturation differ in the positions of multiple bonds, the senior array is that having multiple bonds with the lowest locants;

(c) the array with the largest number of substituents;

(d) the array having substituents with the lowest locants;

(e) the array in which the substituent first in alphabetical order has the lowest locant.

Carbocyclic Ring Systems. Among carbocyclic ring systems, the decreasing order of seniority is as follows:

(a) a ring system containing the largest number of rings;

(b) a ring system with the largest individual ring at the first point of difference;

(c) a ring system having the largest number of atoms common to the rings;

(d) a ring system with the lowest numbers at the first point of difference for ring junctions.

The order of decreasing seniority for a given carbocyclic ring system is as follows:

(a) when two carbocyclic systems differ only in degree of unsaturation, the senior system is that with the lowest state of hydrogenation;

(b) when two carbocyclic systems of the same degree of unsaturation differ in the positions of multiple bonds, the senior system is that having multiple bonds with the lowest locants;

(c) a ring system with the lowest locants of free valences;

(d) in assemblies of identical carbocyclic systems, the assembly of highest seniority is that having lowest numbers for the points of attachment between the systems within the assembly consistent with the fixed numbering of the systems;

(e) a ring system with the largest number of substituents;

(f) a ring system having substituents with the lowest locants;

(g) a ring system in which the substituent first in alphabetical order has the lowest locant.

Acyclic Carbon Chains. Acyclic carbon chain seniority is based on the length of the chain. A longer acyclic carbon chain is senior to a shorter one.

The order of decreasing seniority of acyclic carbon chains of equal length is as follows:

(a) when two chains differ only in degree of unsaturation, the senior chain is that with the lowest state of hydrogenation;

(b) when two chains of the same degree of unsaturation differ in the positions of multiple bonds, the senior chain is that having multiple bonds with the lowest locants;

(c) the chain with the largest number of substituents;

(d) the chain having substituents with the lowest locants;

(e) the chain in which the substituent first in alphabetical order has the lowest locant.

APPENDIX 2. EXAMPLES OF NAMES

(In the examples, a common name of the structure is always followed by its segment name. Comments on the choice of the main chain and/or the direction of citation of segments are given in parentheses.)

1. 9-β-D-ribofuranosyl-9*H*-purin-6-amine (adenosine)

β-D-ribofuranosyl−6-amino-9*H*-purin-9-yl

(O is senior to N)

2. tris(hydroxymethyl)methylamine

2-amino-3-hydroxy-2-(hydroxymethyl)propyl−hydroxy

(longer carbon chain; symmetrical structure, either direction)

3. pentaerythritol

3-hydroxy-2,2-bis(hydroxymethyl)propyl−hydroxy

(symmetrical structure, either direction)

4. pentaerythritol monoacetate

3-hydroxy-2,2-bis(hydroxymethyl)propyl−acetyloxy

(O is senior to carbon chain of acetyl)

5. *N*-(1-chloroethyl)-*N*-ethylbutanamine

1-chloroethyl−*N*-ethylbutylimino

(Cl is senior to carbon chain; butyl longer than ethyl)

6. 1-chloro-*N*-(2-chlorobutyl)-*N*-(3-chlorobutyl)butanamine

3-chlorobutyl−(1-chlorobutyl)imino−2-chlorobutyl

(longest carbon chain between Cl; longer carbon chain between Cl and N)

7. 7-(4-hydrazinobenzeneazo)-1-hydroxynaphthalene-2-sulfonic acid

sulfo−1-hydroxynaphthalene-2,7-diyl−diazenediyl−4-hydrazinophenyl

(OH of SO_3H is senior to N)

8. (9-cyclopentyl-6-cyclopropyldecane-2-yl)cyclohexane

1-cyclohexyl-5-cyclopropyl-1,8-dimethyloctyl−cyclopentyl

(cyclohexane is senior to cyclopentane)

9. 1-ethyl-3-{2-[3-(2-{3-[2-(2-ethylcyclopropyl)ethyl]-cyclobutyl}ethyl)cyclopentyl]ethyl}cyclohexane

3-ethylcyclohexyl−ethane-1,2-diyl−cyclopentane-1,3-diyl−ethane-1,2-diyl−cyclobutane-1,3-diyl−ethane-1,2-diyl−2-ethylcyclopropyl

(ethyl vs ethyl; cyclohexane is senior to cyclopropane)

10. 1-(3-cyclopentylideneimino-2,2-dimethylpropyl)-pyridinium

2,2-dimethyl-3-(pyridinium-1-yl)propyl−cyclopentylideneimino

(pyridinium is senior to cyclopentane)

11. 2-[4-(phenylhydrazino)phenylazo]-1-naphthol

l-hydroxy-2-naphthyl−diazenediyl−1,4-phenylene−phenylhydrazino

(O is senior to benzene)

12. 1-[3-(1-ethyl-7,7-dimethylbicyclo[2.2.1]hept-2-yl)-2,2-dipropylpropyl]-6-[2-(2-ethyl-6-methylcyclohexyl)ethyl]-8-(1-ethyl-6-methylperhydroinden-4-yl)perhydrophenalene

1-ethyl-7,7-dimethylbicyclo[2.2.1]hept-2-yl−2,2-dipropylpropane-1,3-diyl−8-(1-ethyl-6-methylperhydroinden-4-yl)perhydrophenalene-1,6-diyl−ethane-1,2-diyl−2-ethyl-6-methylcyclohexyl

(longer main chain; ethyl vs ethyl, bicyclic system is senior to cyclohexane)

13. 4,4′-{1-[({5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy)-carbonyl]ethylene}dibenzoic acid

carboxy−1,4-phenylene−2-(4-carboxyphenyl)-3-oxopropane-1,3-diyl−oxy−pentane-1,5-diyl−oxy−biphenyl-4,4′-diyl−cyano

(longer main chain; OH in COOH is senior to N)

14. 9-[4,5-dimethoxy-2-[(1,2,3,4-tetrahydro-6,7-dimethoxy-2-methylisoquinolin-1-yl)methyl] phenoxy]-5,6,6a,7-tetrahydro-2,10-dimethoxy-6-methyl-4*H*-dibenzo[*de*,*g*]quinolin-1-ol

methoxy−5,6,6a,7-tetrahydro-1-hydroxy-10-methoxy-6-methyl-4*H*-dibenzo[*de*,*g*]quinolin-9-yl−oxy−4,5-dimethoxy-1,2-phenylene−methylene−l,2,3,4-tetrahydro-7-methoxy-2-methylisoquinoline-1,6-diyl−methoxy

(CH_3O vs CH_3O; dibenzoquinoline is senior to isoquinoline)

15. 2,8-diacetoxy-9-chloro-7-ethyl-10-(3-ethyl-10-fluorodispiro[5.1.7.2]heptadec-17-yl)-4a,6-bis(2-oxoethoxy)-4a,5a,-9a,10a-tetrahydroindeno[1,2-*b*]indole-3-carboxylic acid

2-oxoethyl−oxy−2,8-diacetoxy-3-carboxy-9-chloro-7-ethyl-10-(3-ethyl-10-fluorodispiro[5.1.7.2]heptadec-17-yl)-4a,5a,9a,10a-tetrahydroindeno[1,2-*b*]indole-4a,6-diyl−oxy−2-oxoethyl

(longest main chain)

16. 1-deoxy-1-(3,4-dihydro-7,8-dimethyl-2,4-dioxobenzo-[*g*]pteridin-10(2*H*)-yl)-D-ribitol (riboflavin)

3,4-dihydro-7,8-dimethyl-2,4-dioxo-2*H*-benzo[*g*]pteridin-10-yl−1-deoxy-D-ribitol-1-yl

(O vs O; pteridine is senior to carbon chain)

17. *N*-[4-[[(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)-methyl]amino]benzoyl]-L-glutamic acid (folic acid)

2-amino-1,4-dihydro-4-oxopteridin-6-yl−methylene−imino−1,4-phenylene−carbonyl−imino−1,3-dicarboxypropyl

(longer carbon chain; O vs O, pteridine is senior to carbon chain)

18. 9-β-D-ribofuranosyl-9*H*-purin-6-amine 5′-(trihydrogen diphosphate) 3′-(dihydrogen phosphate) *P*′-mono[(*R*)-3-hydroxy-4-[[3-[(2-mercaptoethyl)amino]-3-oxopropyl]amino]-2,2-dimethyl-4-oxobutyl] ester (coenzyme A)

dihydroxyphosphoryl−1β-(6-amino-9*H*-purin-9-yl)-1,5-dideoxy-D-ribofuranose-3*O*,5-diyl−oxy−hydroxyphosphoryl−oxy−hydroxyphosphoryl−oxy−(*R*)-3-hydroxy-2,2-dimethyl-4-oxobutane-1,4-diyl−imino−3-oxopropane-1,3-diyl−imino−2-mercaptoethyl

(longer main chain; O in phosphate is senior to S)

19. 1-deoxy-1-(3,4-dihydro-7,8-dimethyl-2,4-dioxobenzo-[*g*]pteridin-10(2*H*)-yl)-D-ribitol 5′-(trihydrogen diphosphate), *P*′ → 5′-ester with 9-β-D-ribofuranosyl-9*H*-purin-6-amine (FAD)

3,4-dihydro-7,8-dimethyl-2,4-dioxo-2*H*-benzo[*g*]pteridin-10-yl−1,5-dideoxy-D-ribitol-1,5−diyl−oxy−hydroxyphosphoryl−oxy−hydroxyphosphoryl−oxy−1,5-dideoxy-D-ribofuranose-5,1β-diyl−6-amino-9*H*-purin-9-yl

(O in pteridine is senior to N in adenosine)

20. 2,2′-[methylenebis[oxy(2-oxo-2,1-ethanediyl)]]bis[1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-6,7-dimethoxy-2-methylisoquinolinium]

methoxy−6-methoxy-1,3-phenylene−methylene−6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoquinolinium-1,2-diyl−2-oxoethane-1,2-diyl−oxy−methylene−oxy−1-oxoethane-1,2-diyl−6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoquinolinium-2,1-diyl−methylene−6-methoxy-1,3-phenylene−methoxy

(symmetrical structure; either direction)

21. 1-[2-[(2-ethylhexyl)imino]ethyl]-α-methyl-4-oxo-2,5-cyclohexadiene-1-acetonitrile *N*-oxide

(2-ethylhexyl)oximino−ethane-2-yl-1-ylidene−4-oxocyclohexa-2,5-diene-1,1-diyl−1-cyanoethyl

(O in oximino is senior to both ethylhexyl and N in CN)

22. methyl 2-hydroxymethyl-5-{2-[[1-(hydroxymethyl)-propylidene]amino]ethyl}-4-[2-(methylamino)propyl]-7-(*N*-methylsulfenamoyl)-3-heptenoate thiosemicarbazone

1-ethyl-2-hydroxy-1-ethylidene−nitrilo−6-(hydroxymethyl)-7-methoxy-4-(methylamino−1-methylethane-1,2-diyl)-3-(methylamino−thio−ethane-1,2-diyl)hept-4-en-1-yl-7-ylidene−diazan-2-yl-1-ylidene−thiocarbamoyl

(the longest main chain; O is senior to N, S or C)

23. 4-({2-[*N*-(4-aminobenzyl)-*N*-(4-hydroxyphenyl)amino]-2-[(4-hydroxyphenyl)oxy]ethyl}thio)phenol

4-hydroxyphenyl−thio−2-(4-hydroxyphenyl−oxy)ethane-1,2-diyl−(4-hydroxyphenyl)imino−methylene−4-aminophenyl

(longest main chain containing most acyclic C and heteroatoms, O is senior to N)

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CI950202S