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## ON THE NOMENCLATURE OF OLIGOFLAVANOIDS WITH AN A-TYPE UNIT

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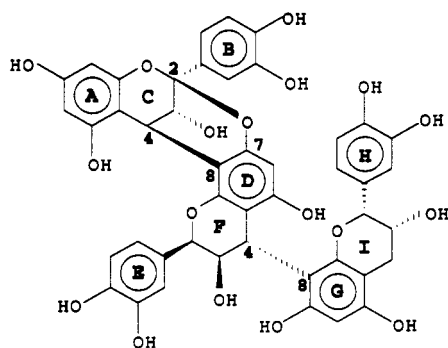
**ABSTRACT.**—Configurational assignments at C-4 of proanthocyanidins denoted by the  $\alpha,\beta$  nomenclature lacks correctness once a unit has been rotated through  $180^\circ$  as feasible in oligoflavanoids with an A-type unit.

Owing to the growing need for a convenient but accurate system of nomenclature for naming proanthocyanidins, Hemingway and co-workers (1,2) recently introduced a form of nomenclature analogous to the IUPAC system for naming oligo- and polysaccharides which appears neat and exceedingly attractive. This straightforward system of nomenclature for this polyphenolic group of plant metabolites was subsequently extended for general application (3) and is now commonly used in this field.

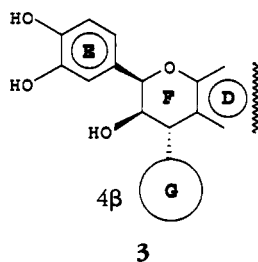
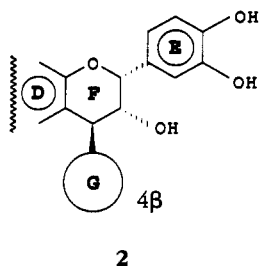
Briefly, in this system the basic flavan structural unit of oligomers is defined in terms of the familiar monomeric flavan-

3-ols for the  $2R$  isomers, distinguished by the prefix *ent* from the less common  $2S$  isomers (4). The corresponding  $3\alpha$ -OH isomers in each series are indicated by adding "epi" to the beginning of the appropriate monomer name. The configuration of the interflavanoid bond at C-4, which is equivalent to the anomeric C-1 of a sugar unit in oligosaccharides, is denoted by the  $\alpha,\beta$  nomenclature (4) within brackets as in the carbohydrates.

Although the above system is well suited for naming complex oligoflavanoids precisely, some inconsistencies demand nomenclatural reappraisal. One concern is the fact that definition of the stereochemistry ( $\alpha$  or  $\beta$ ) of the interflavanoid bond of trimeric and of higher oligoflavanoids with an A-type unit has thus far been incorrect with the exception of the paper by Tanaka *et al.* (5). The pitfalls in defining the C-4 stereochemistry of, e.g., the "middle" unit in such trimers are quite clear. As illustrated in structure 1, the DEF unit is a  $4\beta$ -substituted (–)-epicatechin unit despite the fact that it has been rotated through  $180^\circ$  in comparison to the way in which it is normally presented. As presentations 2 and 3 both reflect a  $4\beta$ -substituted (–)-epicatechin unit, one is thus allowed to present the "middle" unit as in 3, but when allocating configuration at C-4 the flavanyl unit should always be viewed as



1



in the "conventional" manner of **2**. This clearly follows from rule F-6.2 (4): "Whenever this system is used, the orientations depicted in these Rules for the parent structure *must be retained*." Trimer **1** is accordingly epicatechin-(2 $\beta$ →O→7,4 $\beta$ →8)-epicatechin-(4 $\beta$ →8)-epicatechin rather than epicatechin-(2 $\beta$ →O→7,4 $\beta$ →8)-epicatechin-(4 $\alpha$ →8)-epicatechin as was indicated by, e.g., Nonaka *et al.* (6) and Haslam (7).

This is just one example of the hitherto inconsistent application of the  $\alpha,\beta$  nomenclature for such polyphenols. This, of course, implies that either the formulae or the naming of such proanthocyanidins reported to date requires appropriate correction, while taking into account the spectroscopic data again, as in our own work on the proanthocyanidins from *Pavetta owariensis* (8). The relative 3,4-stereochemistry of ring F, for instance, is evident from the coupling constant of heterocyclic protons, while  $^{13}\text{C}$ -nmr and cd data are indicative of the orientation of the interflavanyl linkage (9), thus eliminating discrepancies between structure and naming.

In summary, oligoflavonoids with an A-type unit require special attention regarding configurational assignment at C-

4 by the  $\alpha,\beta$  nomenclature to prevent ambiguities outlined above.

#### ACKNOWLEDGMENTS

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