Division of Carbohydrate Chemistry, American Chemical Society,

and ACS Committee on Nomenclature, Terminology, and Symbols

248th National ACS Meeting
San Francisco, California

Report on Biochemical and Carbohydrate Nomenclature

This report is a brief update on the detailed report presented at the Dallas ACS meeting in March 2014 to the ACS Committee on Nomenclature, Terminology, and Symbols, and to the ACS Division of Carbohydrate Chemistry. It concerns primarily the discussions and actions taken at the meeting in Utrecht, The Netherlands, of the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) during May 12—14, 2014.

Attending the meeting were Gerard Moss (Chairman); Richard Cammack; Kristian Axelsen; Ron Caspi (Secretary); Derek Horton; Masaaki Kotera; Andrew McDonald; Ida Schomburg; Keith Tipton; Hans Vliegenthart (host for the meeting); Shuchismita Dutta; and Observers, IUPAC Division VIII; Ture Damhus; Karl-Heinz Hellwich; Marcus Ennis; Sameer Velankar; and Dietmar Schomburg.

Major topics were enzymes, flavonoids, and carbohydrates. The previous report detailed the ongoing work on *Enzyme Nomenclature and Classification*, and an additional 300 entries into the EC List were reported. Ongoing work on the *Small Molecules Glossary* project focused on substrates and inhibitors of enzymes, free radicals, and on organometallic complexes. The new Blue Book, on Nomenclature of Organic Chemistry, has now appeared. The IUPAC-IUBMB document on *Flavonoid Nomenclature*, previously reported to this committee, was developed by a panel including Amelia Rauter, Derek Horton, Gerard Moss, Bernardo Herold, Karl-Heinz Hellwich, Ida Schomburg, and Marcus Ennis. The document has completed its external review by IUPAC and the final corrections are being incorporated into the document prior to its publication.

Carbohydrate Nomenclature

The expert panel charged with revising the 1996 IUPAC carbohydrate document devoted a long session in Utrecht in making a point-by-point review of the 1996 document (2-Carb) with the view to covering new areas that have arisen, providing new examples, clarifying some of the wording in 2-Carb, discussing symbolic representation of complex structures, and seeking ways to bringing the bioinformatics specialists into a common understanding with the language of the experimentalist.

The carbohydrate panel included the following: J. F.G.Vliegenthart, Derek Horton, Amelia Rauter, G.P.Moss, Karl-Heinz Hellwich, Thomas Luetteke, Martin Frank. Sandro Sonnino and Nuno Xavier) earlier appointed to the panel, were absent.

The panel set out to revise each of the 39 sections in 2-Carb with the target objective of a revised document, identified as 3-Carb. Within the time available, all of the sections through 2-Carb-32 were discussed and revised, and a record of the revisions noted. Considerable work remains to be done on the sections 2-Carb-32 through 2-Carb-39, and this will be undertaken at the time of the next meeting of the panel, tentatively scheduled for May 2015 in Braunschweig, Germany. Some of the items in 2-Carb for detailed discussion and revision are noted here:

2-Carb-36.4 **Trivial names.** This list of trivial names and their systematic equivalents needs to be expanded to more examples.

2-Carb-37 **Cyclic oligosaccharides.** This section requires significant alteration to reflect current usage. The cyclodextrin trivial names should be retained, but the systematic names using the ”malto” infix should be revised, as there are many different linkage-modes known. The “cyclohexakis” and “cycloheptakis” prefixes can be used with the monosaccharide components in any linkage-mode. The literature reports cyclic that have been termed “cyclofructins”. Such names should conform to the accepted “an” suffix for new carbohydrates, and not perpetuate a suffix used for proteins.

2-Carb-38 **Symbolic depiction of oligosaccharide structures.** The extended form 2-Carb-38.3 should be retained as the definitive form, but the “condensed” form 2-Carb-38.4 should be removed, while the “short” form 2-Carb-38.5 should be retained for use when the ring size and enantiomeric identity of the monosaccharides are independently defined. The “short” form provides a direct connection to the iconic presentation recommended by the Consortium for Functional Glycomics (see examples to be presented) and which is recommended for adoption in 3-Carb.

2-Carb-39. **Polysaccharides.** This section requires significant expansion to incorporate many more examples of commercially important polysaccharides, as well as acceptable ways to name synthetic modification of such natural polysaccharides.

2-Carb-39.9 **Glycoproteins, glycopeptides, and peptidoglycans**. These need a full section on their own, with major augmentation and depiction along the lines of the N-glyco-tetrapeptide example supplied, displaying a glycopeptide of 25 monosaccharides attached to a tetrapeptide, with the oligosaccharide displayed both as a full conformational formula and in the iconic system noted in 2-Carb-38. The two examples of neoglycoproteins need major supplementation to illustrate new linkers between the carbohydrate and protein, notably the triazole linker.

In the **Appendix**, the lists of trivial names need to be augmented. The **Glossary of Terms** in 2-Carb has been very well received and should be retained, as is, in 3-Carb.

Submitted by Derek Horton.