

In the depth of oligosaccharidic structural complexity: The example of multiply branched glycans

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Due to their highly chiral nature and the large variety in glycosidic sequences, Glycans are clearly amongst the most complex families of biological compounds. Post-transcriptional modifications or enzymatically chiselled polysaccharides can lead to extreme diversity in glycanic sequences. This is particularly true in the case of branched oligosaccharides. Starting from a reducing extremity or an aglycone moiety the addition of each supplementary carbohydrate unit will result in a geometric multiplication of potential unique tridimensional glycanic structures. In the presented example in a glycan constituted of only one type of sugar, glycosylated through only two (m) or (i) positions, the number of discrete structures obtained by the addition on any of the (m) or (i) available branching sites of the parent glycan will increase tremendously with each added sugar residue. The addition of each supplementary sugar unit will follow a combinatorial development. At each degree of polymerization DP(n) the number of potential isomer N of DP(n) will be as follows $N(n) = 2n - 1 + [(n-2) + 2n-3 * (n-3)] + [(n-3 + 2n-3 * (n-3)] + [n-4 + 2n-4 (n-3) \text{ etc..}$. Thus for each increment of the DP (n), the number of potential discrete structures in each DP groups can be calculated as $(2n \text{ choose } n)/(n+1) = (2n)!/(n!(n+1)!) [1]$ in a pattern first addressed by the mathematician E. C. Catalan [2] who described in the 19th century the combinatorial development of such binary trees. As a result the number of potential isomeric forms for such branched oligosaccharidic structures is given by a Catalan number C_n , going from two isomers for the disaccharides to 16796 isomers for a deca-saccharide. The example of deciphering the branched glycanic mixtures of hydrolysed reserve polysaccharides [3] will be presented.

[1] Jean-Christophe Aval, Multivariate Fuss–Catalan numbers, Discrete Mathematics 308 (2008) 4660 – 4669.

[2] E. C. Catalan, Note sur une équation aux différences finies, J. Math. Pures Appl. 3 (1838) 508-516. & (ibid) 4 (1839), 91-94.

[3] Bliard, C., Martinez, A. (2008). Analyse prédictive des structures potentielles des dextrines MOS et MIMOS. "SCF Grand Est V" Fifth meeting of the SCF GE. Vandoeuvre les Nancy, France, 15th of April.