Sweet Pages

Have you ever wondered what types of structures are hidden behind the sequence specifications commonly used in carbohydrate chemistry, such as α-D-Gal*p*NAc-(1→3)-[α-L-Fuc*p*-(1→2)]-D-Gal*p*? You will find the answer on the home page of the German Cancer Research Center's (DKFZ, Heidelberg) molecular modeling group headed by C.-W. von der Lieth. Starting from a frugal entrance page, a multitude of services and information for those interested in glyco sciences is accessible.

The program SWEET-II[1] is probably the most interesting application for the visitor of the site. Starting from the common sugar nomenclature, SWEET-II generates 3D structures of the entered oligosaccharides in a single possible conformation. The sequence of a carbohydrate is entered into a form which is available in several modes adapted to the user's experience. It is possible to enter simple disaccharides but also complicated branched oligosaccharides and glycoconjugates, such as glycopeptides and -lipids, or even cyclodextrins. Those not familiar with sugar nomenclature may click on pre-assembled biologically relevant oligosaccharides. SWEET-II links pre-constructed monosaccharide templates and subsequently optimizes each glycosidic bond. The structure is then optimized by using Allinger's MM3 force field. The resulting output can be obtained in PDB or VRML format. Several methods for visualization are available. Using the freely available plug-in Chime for example, you can rotate and scale the molecules and examine them from any perspective. The structures generated by SWEET-II are considered by the authors to be "preliminary but reliable" and they are suited as useful starting points for further refinements.

PDB files generated by SWEET-II or obtained from any other source may also be used as input for another program, PDB2MultiGIF,[2] which converts Cartesian coordinates to animated GIF images of rotating molecules. Visualization parameters may be set by the user. Basic knowledge of the visualization program RASMOL is helpful in this respect.

Another application which is potentially of high value for glycobiologists is the database SWEET-DB.[3] This database, which is still under construction, is an attempt to link information on glycans available from different sources through a unique description of their chemical structure (Linear Notation for Unique Description of Carbohydrate Sequences, LINUCS). Currently, SWEET-DB contains about 50000 oligosaccharide structures taken from CarbBank[4] and 1600 ^{1}H and ^{13}C NMR spectra from SugaBase.[5] Spatial coordinates generated with SWEET-II and optimized with MM3 as well as links to PubMed and the German literature delivery service Subito were added. You can also search for (sub)-structures and bibliographic data. Since the user interface of SWEET-DB is currently renewed, it was not yet possible to look up NMR data again when this review was written. Unfortunately, the database is also not completely up to date. The most recent publications are from 1999, the year in which CarbBank was shut down. However, methods are currently developed to update SWEET-DB so that in the future, an extremely interesting information source is to be expected.

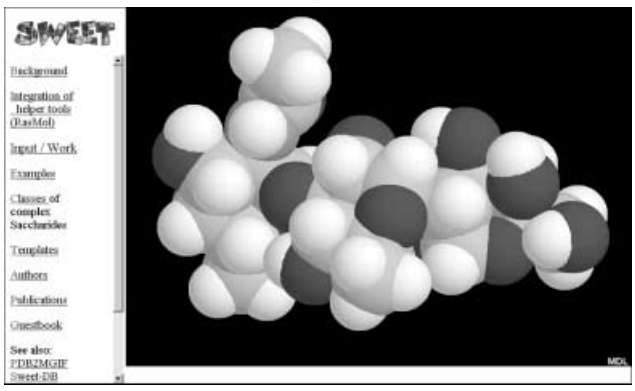

Figure 1. Easily obtained structure of α-D-Gal*p*NAc-(1→3)-[α-L-Fuc*p*-(1→2)]-D-Gal*p*.

Finally, some accessories are offered at the web site, such as programs for the conversion of torsion angles and for the analysis of mass spectra of glycoproteins, as well as many useful links regarding carbohydrates, molecular modeling, and software.

Suggest a web site or submit a review:
angewandte@wiley-vch.de

Who is the addressee of this page? The structures generated by SWEET-II are probably used primarily for teaching and illustration purposes; especially SWEET-DB might become an important tool for researchers in the field of glycomics. A similar database is developed by the Consortium for Functional Glycomics,[6] in which the modeling group from Heidelberg participates. By the way, the trisaccharide mentioned at the beginning is the blood group A antigenic determinant.

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[1] A. Bohne, E. Lang, C.-W. von der Lieth, *J. Mol. Model.* **1998**, *4*, 33-43.
[2] A. Bohne, *J. Mol. Model.* **1998**, *4*, 344-346.
[3] A. Loß, P. Bunsmann, A. Bohne, A. Loß, E. Schwarzer, E. Lang, C.-W. von der Lieth, *Nucleic Acids Res.* **2002**, *30*, 405-408.
[4] S. Doubet, K. Bock, D. Smith, A. Darvill, P. Albersheim, *Trends Biochem. Sci.* **1989**, *14*, 475-477.
[5] J. van Kuik, K. Hard, J. F. Vliegenthart, *Carbohydr. Res.* **1992**, *235*, 53-68.
[6] http://glycomics.scripps.edu/

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