

Project Summary

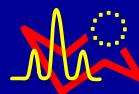
Carbohydrates are involved in a variety of fundamental biological processes, e.g. cellular differentiation, embryonic development and fertilization. They are also involved in numerous pathological conditions such as e.g. bacterial and viral infections, inflammatory diseases and cancer and therefore offer attractive pharmaceutical and diagnostic applications.

In contrast to the genomic and proteomic area, no large data collections for carbohydrates have been compiled so far. The availability of such comprehensive databases, however, will be a prerequisite to successfully perform large-scale glycomics projects aiming to decipher new, so far unknown biological functions of glycans. For this purpose, common protocols and quality criteria for the generation of experimental data and guidelines of good practise for the establishment of databases are indispensable, especially for NMR-, MS- and HPLC-data, which are the key technologies for the identification and analysis of carbohydrates.

The Internet offers the unique chance to constitute a global and interactive peer-to-peer communication for scientific data. The outlined initiative aims to provide a tool for streamlining European research in glycobiology through the development of bioinformatics standards, databases, algorithms and software components. To guarantee maximal synergetic effects other available bioinformatics and biomedical resources will be linked to the newly created databases and cross-referenced in an efficient way.

The interpretation of MS- and NMR spectra as well as HPLC profiles of glycans is extremely complicated without appropriate reference data. The development of appropriate algorithms, which enable a rapid and reliable automatic annotation and interpretation of MS- and NMR-spectra, is a major aim of this design study. This effort is comparable to the automation of nucleic acid sequencing that enabled the large scale genomics studies and will lead to a comparable impetus for glycomics.

Group of Experts



General Concepts

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Design Studies

Related to the Development of

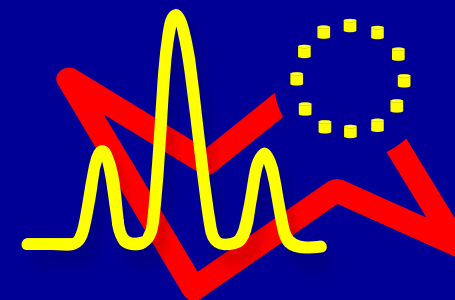
Distributed, Web-based

European

Carbohydrate Databases

for Primary

Experimental Data

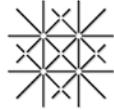


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EUROCarbDB Partners



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Department of
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Oxford Glycobiology Institute
University of Oxford

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EUROCarbDB is a Research Infrastructure Design Study Funded by the 6th Research Framework Program of the European Union
Contract: RIDS Contract number 011952



GlycoPeakfinder is a tool for fast annotation of glycan MS spectra. MS-profiles, MSn spectra with different types of ions (glycosidic cleavages and/or cross-ring cleavages) can be calculated in parallel. The option of detecting differently- and/or multiply-charged ions in one calculation cycle provides a fast and complete annotation of the whole spectrum. All the additional options of „Glyco-Peakfinder“ (e.g. calculation of modifications either at the reducing end or within the sequence) increase the field of application from native glycans to a variable set of glycoconjugates.

Mass	Intensity	Composition (check for fragment and structure search)	Charged ions	Ion type	Mass calculated	Deviation [ppm]
421.200	n/a	Hex2-PA	H+	Y	421.18167	-43.5
443.100	n/a	Hex2-PA	Na+	Y	443.16362	143.6
459.200	n/a	Hex2-PA	K+	Y	459.13755	-136.0
527.300	n/a	Hex3	Na+	C	527.15825	-268.8
543.200	n/a	Hex3	K+	C	543.13219	-124.8
1069.600	n/a	Hex6-PA	H+	Y	1069.39296	-193.6
1091.600	n/a	Hex6-PA	Na+	Y	1091.37491	-206.2
1107.600	n/a	Hex6-PA	K+	Y	1107.34884	-226.8
1393.800	n/a	Hex8-PA	H+	Y	1393.49861	-216.2
1415.700	n/a	Hex8-PA	Na+	Y	1415.48055	-155.0

Mass: 1849.7206 Da [MONO,Und,H+]

GlycoWorkbench is a suite of software tools designed for rapid drawing of glycan structures and for assisting the process of structure determination from mass spectrometry data. The graphical interface of GlycoWorkbench provides an environment in which structure models can be rapidly assembled, their mass computed, their fragments automatically matched with MSn data and the results compared to assess the best candidate.

The **EUROCarbDB web-site** offers an open forum, where all questions concerning standardisation of glycan-related databases, informatics for glycobiology and glycomics as well as data exchange formats will be discussed. It offers a unique chance to meet the experts, to discuss your own ideas and to be informed about ongoing projects.

Topics	Replies	Author	Views	Last Post
Glycans - Glyde (enlargements)	6	Bend Ranzinger	40	Fri Aug 12, 2005 8:33 am Boland Stenzel
Glycans	0	Willi von der Lieth	35	Mon Jul 04, 2005 1:52 pm Willi von der Lieth
Glycans with more than 6 carbons	0	Thomas Lütke	30	Mon Jun 13, 2005 9:03 am Thomas Lütke
Monosaccharide Residue Notation	0	Willi von der Lieth	45	Sun Jun 12, 2005 3:11 pm Willi von der Lieth