

NEWSLETTER

2006/01

Let's put the train together!

Increasing awareness for the need of databases for glycomics and glycobiology

The release of the first EUROCarbDB newsletter falls into an active period of events highly relevant for the future of glyco-related databases:

The European Science Foundation Statement has published a statement "Structural Medicine: The Importance of Glycomics for Health and Disease" (see www.eurocarbodb.org), which emphasizes the need to further develop glyco-related databases.

In September 2006, the NIH organised a workshop 'Frontiers in Glycomics' (see report in this issue). The workshop was the largest meeting focused on the development of databases and informatics for glycomics and glycobiology. The list of speakers read like a who's who of bioinformatics for glycomics.

The outcome of this meeting was on the one hand an agreement to a standard exchange format for glycan structures called GLYDE-CT. On the other hand a list of the most urgent needs – top priority has a centralised, comprehensive and highly curated carbohydrate structure database - was compiled and will be published soon as a white paper.

The European Strategy Forum for Research Infrastructures (<http://cordis.europa.eu/esfri/>) published a roadmap emphasising that "*modern science is inconceivable without recourse to well structured, continuously upgraded (...) and freely accessible databases (...). The bioinformatics infrastructure (...) will continue to expand requiring successive investments for major upgrades, and will remain the depository of biological information for as long as we now can foresee*". The concept of EUROCarbDB fits well into the general perspectives of this roadmap.

All the major glycomics initiatives expressed during the 'Frontiers in Glycomics' workshop their willingness to collaborate with each other and work together on the integration of their individual resources into a larger database.

Latest News

Quite recently FDA has approved AFP-L3, the fucosylated AFP as a tumour marker for primary hepatoma which is relatively specific because approximately 95 % of patients with primary hepatoma gave high value of this marker and able to distinguish from the patients with the cirrhosis which is pre-cancerous stage. This is really a break through for the tumour markers in terms of usage of sugar chains as a biomarker.

The EUROCarbDB project will play a leading role within this international concert: it will coordinate the conversion of CarbBank data to GLYCO-CT format as necessary preparatory steps to establish the centralised glycan structure database.

The EUROCarbDB design study is in its second year of funding. The first software tools are now made available to the scientific public. These newly developed and unique software pieces – GlycoPeakFinder and GlycoWorkbench - concentrate on the most urgent need in glycomics: the development of user-friendly and robust tools for the automatic interpretation and annotation of MS spectra. Several other software components and basic databases are currently under development and we will subsequently make them available through the EUROCarbDB home page. For those who want to follow the discussion and developments more closely, we recommend to register for the EUROCarbDB forum (www.eurocarbodb.org) as well as the newsletter, which will appear at least every half a year in the future.

Let's put a first EUROCarbDB train together, so that it can soon leave the station.

Willi von der Lieth



EUROCarbDB

Informatics for Glycomics starts to come of age

some insights from the 'Frontiers in Glycomics: Bioinformatics and Biomarkers in Disease' workshop held September 10-13, at NIH, Bethesda, MD, USA



The workshop and its outcome are remarkable in several aspects:

a) The workshop was the largest meeting focused upon the development of databases and informatics for glycomics and glycobiology. The list of speakers read like a who's who of bioinformatics for glycomics. Thought leaders representing all of the major worldwide projects were invited, and gave comprehensive overviews of what technologies already available. A hot topic for a number of groups was the development of bioinformatics platforms and analytical techniques for the discovery glycans. The slides of all speakers are now available at the URL <http://glycomics.scripps.edu/NIHBioMarker/BioMarkerProgram.html>.

b) The collaborative spirit of all the major glycomics initiatives was highlighted in the bioinformatics sessions. This spirit is exemplified by the support for cross-institutional collaboration on the development of efficient data exchange formats, and in particular GLYDE-CT. An agreement was reached to continue the development of the GLYDE-CD format as an exchange format for glycan structures. Discussions surrounding the development of this standard can be found at the EUROCarbDB forums. In addition, a number of initiatives exhibited a readiness to open access to their individual resources and integrate them into a newly to be generated carbohydrate structure database (see below).

c) The workshop also saw the meeting of leading scientists from the informatics and glycan biomarker discovery area. Currently, there is limited glyco-informatic support for

enhancing the discovery of biomarkers. Nevertheless, it is obvious that rapid progress in this area of research will depend heavily on tools for automatic and reliable interpretation of the vast amount of experimental data generated. There is especially a need to have solutions at hand, which can reliably identify the significant differences between healthy and diseased states of probes. The availability of freely available, robust and comprehensive databases is fundamental to the achievement of these goals. Currently the development of efficient and dependable automatic assignment of glycans on the basis of MS measurements is hampered by the paucity of available MS data for glycans.

d) There was a general agreement expressed by many speakers, that there is an urgent need for a unified, thoroughly curated and sustainable database for carbohydrate structures in biological samples. There is currently no location where information about all carbohydrates reported in refereed scientific papers is systematically stored. This lack of appropriate databases is regarded as the biggest defect in glycomics and glycobiology research. "We need to be able to search databases for what is out there. Imagine genomics and proteomics without GenBank" (Ajit Varki).

Such a central database requires robust manual annotation and curation tools in the hand of qualified experts in glycan structural analysis. The current state-of-the-art in data stored in glyco-related databases reflects a gap of more than 10 years of accumulated knowledge, following the termination of CarbBank in the mid 90s. It will be a major effort to close this gap.

The mightiness of such a project is clearly beyond the scope of the existing larger initiatives in US, Japan and Europe. Additional endeavours, which require extra funding, have to be undertaken to establish and to maintain a central carbohydrate structure database. The new repository should be closely associated with a well-recognized international non-profit academic organisation that provides open access to biological and experimental data.

e) To smooth the way for central carbohydrate structure database the existing larger initiatives agreed to immediately start with the necessary preparatory steps for the conversion of CarbBank data into the GLYDE-CT format. This will be a multi-institutional, international effort, which will be coordinated by the EUROCarbDB / GLYCOSCIENCES.de initiative. However, the success of this project will depend on the collaboration of all involved partners. The result of the new conversion of CarbBank will provide a clean dataset of fully determined glycan structures in GLYDE-CT format. This data set will constitute the state-of-the-art repertoire of available digital glycan structures. These structures will also constitute the foundation for the future centralised database.

f) There are other important tasks, which can be best organised through a collective effort from the glycosciences community. Important aspects are the formulation of a quality measure (Gold Standard) for the intake of structures into the centralised database. An even larger collaborative endeavour for which the input of community is strongly required, are the definitions and guidelines of quality / reliability factors which need to be assigned for all the varying experimental data, and made available through the distributed network.

The internet offers a unique chance to constitute a global and interactive communication net for scientists and for scientific data, through which at least part of the required curation process of databases may be distributed around the world and assigned to groups of experts in different areas (N-glycans, GAGs, etc.). Another attractive idea is to install an expert moderated Wiki for glycobiology, tied closely to structural and experimental data.

g) There was a general agreement that the volume and diversity of glycomics data makes it necessary to distribute it in different locations throughout the world. This approach allows those having the technical expertise required for data generation to maintain close ties with the data and its curation. Furthermore, a comprehensive collection of data processing tools must be available to interpret and mine the data. Maintenance of this tool collection at a single site would be difficult, but these tools can also be distributed over multiple sites that are maintained by the tool developers themselves. This distributed approach makes it necessary to transmit data over the internet when it is being used for biomarker discovery or other purposes. Such a system can work only if robust standards for data transmission are developed and accepted by the scientific community. The development of a standard format for the exchange of glycan structural data over the Internet was recognised as a primary requirement for biomarker discovery by the workshop participants.

In summary: the Frontiers in Glycomics meeting can be regarded as an important milestone for setting priorities for the most urgent steps to tackle the development of databases and informatics for glycomics. There was a clear consensus that the most urgent demand is the establishment of a centralised, well-curated database of carbohydrate structures. Although such a project is clearly beyond the scope of the currently existing worldwide initiatives, there was a willingness of most of the major glycomics initiatives to share their data and other resources to prepare the creation of the centralised resource. To establish the resource itself, additional funding from larger international funding agencies is required.

Regarding the impact of EUROcarbDB at this meeting, one can clearly say that our initiative plays a prominent, if not leading role within the international arena. This role is well documented through our essential contributions to the formulation of GLYDE-CT format in its details. It was agreed to that essentially the GLYCO-CT namespace developed by DS1 members of EUROCarbDB will be adopted for GLYDE-CT. Another indicator of the leading role of EUROcarbDB is the acceptance of the other initiatives, and that EUROCarbDB / Glycosciences.de will coordinate the conversion of CarbBank data to GLYCO-CT format as necessary preparatory steps to establish the centralised glycan structure database. Also the creation of distributed resources to make primary experimental data available through networks follows extensively the ideas and concepts of a peer-to-peer concept as currently being worked on by the EUROCarbDB project. Our project is unique in this respect.

The NIH has assigned six well-known specialists to form a focus group. The task of this group is to condense the results of the meeting and compile a prioritised list of necessary next steps and projects, which are highly required to favour rapid progress in glycomics research. A white paper will be the outcome of the discussion of the focus group. It is the hope that the statements and recommendations made here will guide the NIH authorities for future directions to proceed. Two EUROcarbDB members, Pauline Rudd and Willi von der Lieth are members of the focus group.

Willi von der Lieth,

Coordinator of the EUROCarbDB Project

The spirit of open access is crucial ...

by Willi von der Lieth

Open access means the free online availability of digital content without any barrier like registration with a password. Open access is of paramount significance to establish successfully a network of federated databases as aimed at by the EUROCarbDB project.

EUROCarbDB follows the general lines as established by the European Bioinformatics Institute (EBI) as well as the American National Centre for Biotechnology Information (NCBI) to provide freely available data and bioinformatics services to all facets of the scientific community in ways that promote scientific progress. This is especially true for primary experimental data like MS-, NMR- and HPLC data.

Open access in glycosciences

The idea of free sharing of research data with other colleagues, which is a fundamental agreement in genomics and proteomics research, seems to be not yet fully accepted by the glycosciences community. There are several academic groups as well as companies, which obviously have collected larger amount of unique data relevant to the field, which they explicitly do not want to share because of commercial interests. Seeing this during the NIH "Frontiers in Glycomics" meeting (see report in this newsletter), Pavel Pevzner, professor of bioinformatics at University of California, San Diego, stated that the glycosciences community – at least to some extent – is a rather closed society which has no broader awareness in sharing data for the promotion of scientific progress. Professor Pevzner concluded, that it does not make much sense for him to start research in glycosciences under these conditions.

The EUROCarbDB partners are aware that part of their job promoting the idea of federated databases in glycosciences will be to convince colleagues that it is indeed profitable to deposit their scientific data in well-organised databases and make it freely available to all interested scientists, despite of the additional time they have spent for documentation and annotation. To start this task we summarize here how the open access philosophy increases the chances to promote scientific progress and which might be the advantages for individual researchers.

Data sharing achieves many important goals for the scientific community:

- supporting studies on data collection methods and measurement
- permitting the creation of new datasets by combining data from multiple sources. Bioinformatic databases of genes and proteins have shown, that the linking of data originating from various resources comprehend many synergetic effects.

- promoting new research, testing of new or alternative hypotheses and methods of analysis
- reinforcing open scientific inquiry
- encouraging diversity of analysis and opinions
- facilitating education of new researchers
- enabling the exploration of topics not envisioned by the initial investigators

From the viewpoint of software development the lack of freely available primary experimental data in glycosciences, hampers significantly the development of efficient, robust and reliable algorithms for the high-throughput analysis of glycans. This statement is especially true for the annotation and interpretation of MS spectra.

Everyone benefits (from data sharing), including investigators, funding agencies, the scientific community, and, most importantly, the public. Data sharing provides more effective use of resources by avoiding unnecessary duplication of data collection. It also conserves research funds to support more investigators. The initial investigator benefits, because as the data are used and published more broadly, the initial investigators reputation grows. (Taken from NIH Data Sharing Policy)

The EUROCarbDB idea of federated databases

The EUROCarbDB partners are convinced that creating a grid of distributed local databases will encourage scientists to input their recorded spectra into a local data base and keep it private until it is published. Thus, the open architecture of the database will enable that mirrors can be easily installed at various locations. Inexpensive hardware platforms and the availability of free software tools will favour this process. Experiences from open source projects indicate that also the quality of the provided data will increase. People who have recorded the data will also input and maintain it. The correction of faulty information will be quick, since nobody likes to bear the blame having made available bad data. Looking at the development of other open access data collections, it can be anticipated that free access to spectroscopic data will encourage scientists to create their own applications based on the data provided. The availability of standard exchange format will also accelerate the exchange of information and knowledge (taken from the initial EUROCarbDB application).

We are in complete agreement with Ajit Varki's statement made at the NIH "Frontiers in Glycomics" meeting: *"The spirit of open access is crucial for the development of a centralised carbohydrate structure database. The most open databases will have the most influence in the final database"*

How to judge the quality of experimental data in glycosciences?



Invitation to help establishing reasonable scoring schemata for the quality of MS- and HPLC data

The MS- and HPLC experimentalists of EUROCarbDB have worked hard and collected a rather comprehensive list of measures and criteria for the various experimental techniques, which can be used to assign reasonable scoring schemata. These efforts have resulted in two questionnaires for MS and HPLC data. The NMR questionnaire will follow soon. To be sure, that we have not overlooked possible measures and to guarantee a broad acceptance of the quality criteria within the glycosciences community, the EUROCarbDB steering committee decided to actively distribute questionnaires to other well-known labs for glycan analysis using MS- and HPLC techniques.

Additionally, we invite all interested colleagues to help us to establish reasonable scoring schemata for the quality of experimental data, by filling out the questionnaires carefully. This will help us to make the deposited data more useful from the user's point of view. Having a reasonable scoring in hand, the user will have the choice to look at high-quality data separately, or at all data within a given quality range or include all data deposited, even those which are of low quality. In such a way EUROCarbDB will be able to intake experimental data of varying quality and comprehensiveness and let the choice which data to retrieve and to look at to the user.

The questionnaires are available at the URL:

MS: <http://www.eurocarbdb.org/recommendations/mass-spec-data>

HPLC: <http://www.eurocarbdb.org/recommendations/hplc-data>

The determination of glycans in all its structural details is still a cumbersome task and the reliability of the results depend essentially on many factors like the experimental method applied, the resolution of the recorded spectra as well as the methods used for sample preparation. Often glycans cannot be characterised as stoichiometrically defined molecules e.g. Glycosaminoglycans (GAGs) - where modifications of the basic carbohydrates may be statistically distributed within the polymer.

Therefore, it is not surprising that one of the first questions always arising when discussing the challenge to include primary experimental data into databases is, which data should be included and how to describe the quality and reliability of provided data. This is indeed a broad and open field for discussions, since no standards really exist and only a few attempts have been made so far to address these questions in a systematic way.

No generally accepted and standardised quality criteria exist

It is one of the major aims of the EUROCarbDB design study to work out quality scores for MS- and NMR- spectra as well as HPLC profiles, which have to be assigned before experimental data is entering the database. Our preliminary experiences based on the discussion among the experimentalists within the EUROCarbDB project clearly showed that generally accepted and standardised quality criteria obviously do not exist. Different labs apply different often not clearly defined schemata. Additionally, we had difficulties to come to a consensus, which type of experimental data EUROCarbDB will take in. One extreme position was to accept only high quality data of pure and completely assigned compounds. The other extreme was to take in all available data without any restrictions.

In between these two extreme positions lies the idea to intake all those data, which fulfil certain quality criteria according to a clearly defined scoring scheme. However, we have the immediate problem that no such commonly accepted quality scheme exists, that there are various thinkable criteria, which may be suitable, and that no systematic evaluation of such measures has been performed so far.

First EUROCarbDB annual meeting

Hinxton, UK



Willi von der Lieth, coordinator of the EUROCarbDB project, is handing over the first year report to Jean-Emmanuel Faure, the representative of the European Union.

EMBL
European
Bioinformatics
Institute





Willi and Kim Henrick, leader of the MSD group at EBI and host of the meeting.

Day one ... internal affairs



Pauline Rudd, Louise Royle and Matthew Campell representing HPLC in the project.



Hans Kamerling and Stephan Herget discussing nomenclature of carbohydrates.



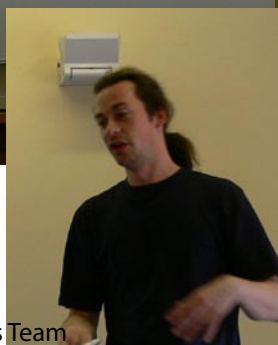
Göran Widmalm, new leader of EUROCarbDB-DS4, is discussing NMR aspects of the project with Bas Leeftang, Rasmus Fogh (CCPN) and Willi von der Lieth.

Day two ... meeting partners

complete meeting program available at <http://www.eurocarbdb.org/about/meetings/programs>



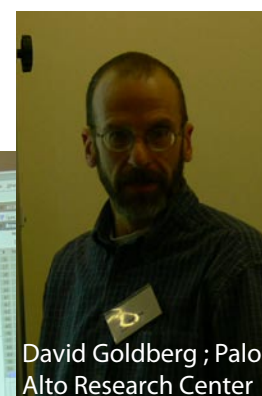
Stuart Haslam, Consortium of Functional Glycomics, Director Analytical Core



Chris Taylor, EBI Proteomics Services Team



Rasmus H. Fogh, CCPN Project



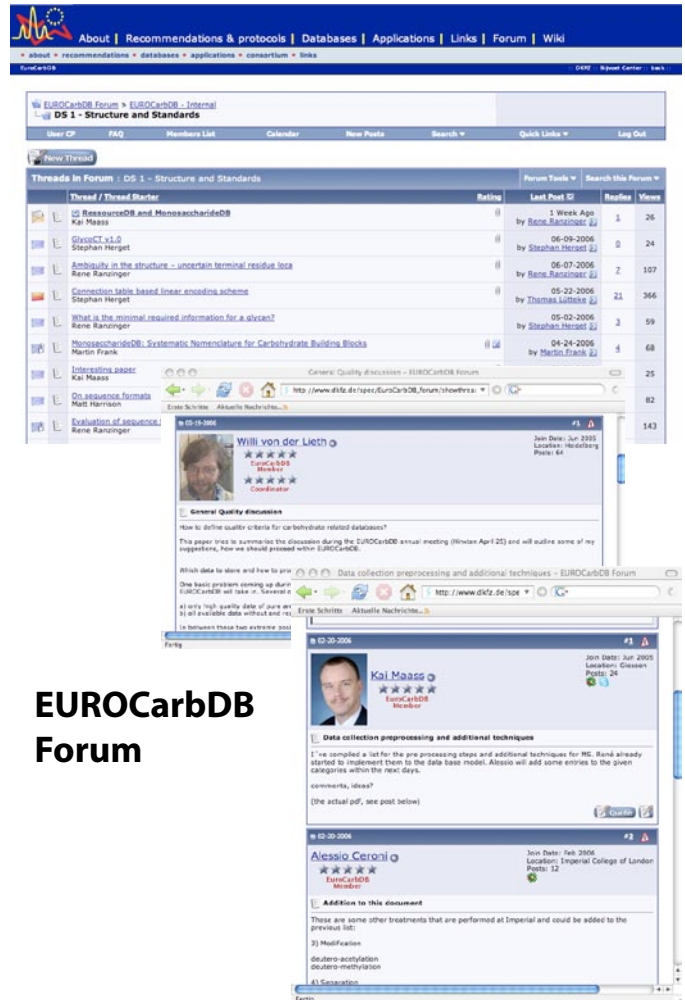
David Goldberg ; Palo Alto Research Center

Moving forward as an international team

The development of bioinformatics standards, databases, algorithms and software components for glycobiology in an international team starts already with facing the challenge to organize efficient ways of communication between the EUROCarbDB developers as well as the glycoscience community. For this purpose we setup a virtual communications centre (*Forum*) that can be accessed following the link 'Forum' of the main menu of the EUROCarbDB homepage. The Forum is intended to be the primary place for discussion and exchange of actual information within the consortium, discussion with experts and other scientist interested in the project. Since the EUROCarbDB forum, although well organized, holds probably to much information (already 432 posts, 76 Threads in the first eight months) for a person not permanently following the ongoing discussions, the more static pages of the EUROCarbDB homepage will help to easily access the outcome of the project (recommendations, tools, etc.) and to follow the major progress made within the consortium. The Forum is organized in three parts: 'Open discussion', 'Expert groups' and 'EUROCarbDB-internal'. The first section is publicly accessible without registration and allows everybody to participate in the discussion.

Intensive and productive discussions took place already in the expert forum e.g. on standardization of the monosaccharide names, sequence formats and data models.

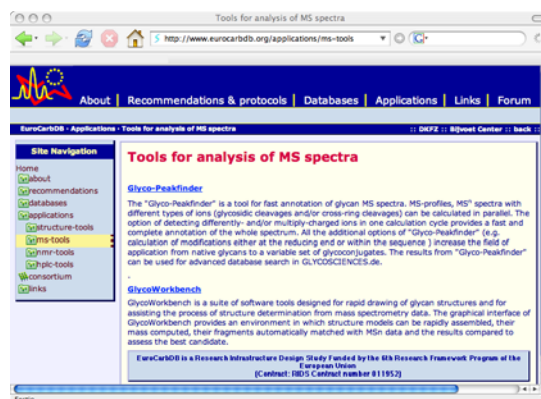
The Forum has also become the primary place for the project management to inform the consortium partners about the decisions made by the steering committee, the agreements and standardizations made by other glycomics projects, to organize meetings and make available the monthly developer reports.



The screenshot shows the EUROCarbDB Forum interface. At the top, there is a navigation bar with links: About, Recommendations & protocols, Databases, Applications, Links, Forum, Wiki. Below this, a user profile for Kai Maass is visible, including his name, role as Coordinator, and location (Gießen, Hesse, Germany). The main content area displays a thread titled "General Quality Discussion - EUROCarbDB Forum" with a sub-header "Data collection preprocessing and additional techniques". The thread content includes a discussion about quality criteria for carbohydrate-related datasets and a list of recommended treatments for MS spectra.

EUROCarbDB Forum

EUROCarbDB Homepage



The screenshot shows the EUROCarbDB Homepage. The main navigation bar is identical to the forum screenshot. The page content is divided into a left sidebar with a "Site Navigation" menu and a main content area. The main content area is titled "Tools for analysis of MS spectra" and features a section for "Glyco-Peakfinder". The text describes this tool as a fast annotation tool for glycan MS spectra, capable of calculating MS-profiles and MSⁿ spectra in parallel. It also mentions "GlycoWorkbench" as a suite of software tools for rapid drawing of glycan structures.



The screenshot shows the EUROCarbDB Reports page. It features a "Reports" section with a list of reports, each with a title and a link to the report. The reports include:

- 001: Experimental techniques for biological data collections in glycomics and digital descriptions used for the representation of carbohydrate structures
- 002: Survey structural complexity of carbohydrates and their profiles of occurrence in various tissues, species and cells
- 003: Concept and implementation plan P2P-network, the central database and storage facilities
- 004: Experimental and digital standards for MS spectra and HPLC
- 005: Guidelines for a uniform description of NMR spectra

 The page also includes a "Site Navigation" menu on the left and a footer with contact information for the European Union.

Developer Meetings

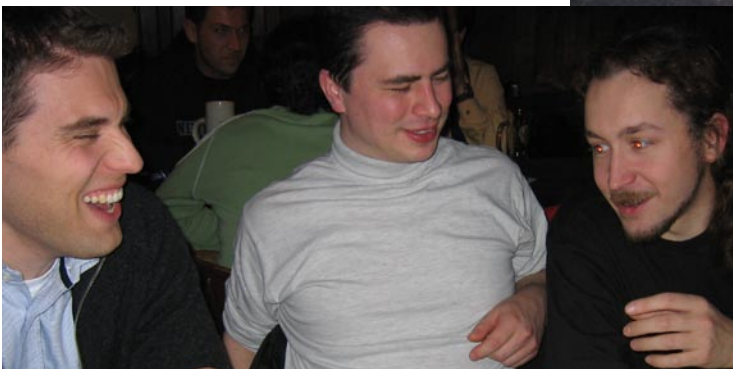
Although discussions in the EUROCarbDB forum were very productive already, there are clear limitations in this approach. Therefore alternative ways how developers can interact were established as well. Several developer 'hands-on' meetings were organized in cooperation with EUROCarbDB partners at different locations since the start of the project. Next to the EUROCarbDB internet forum, VoIP- and video conferences, these meetings have turned out to be the most important cornerstone for efficient project progress: developers can

meet in person, get updated on the status of the several sub-projects and discuss problems in focus groups. Finally, a new task list is compiled during a round table discussion.

As an addition to the Forum a EUROCarbDB Wiki is available where technical information is stored that developers may need for their daily work.



Intensive discussions



...til late at night.



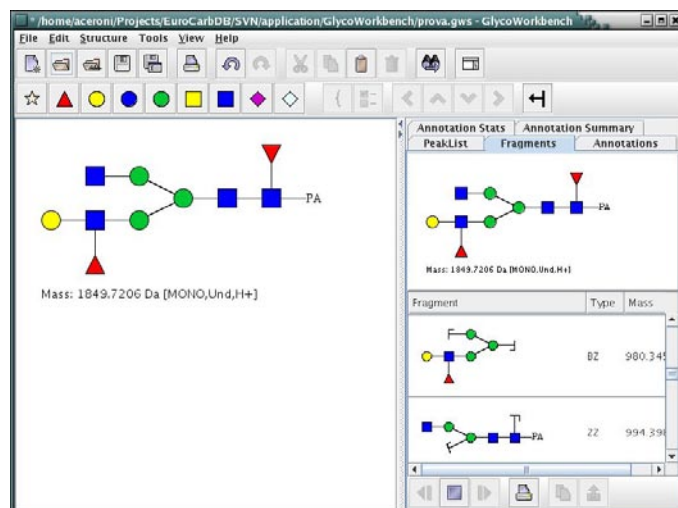
GlycoWorkbench

a Software Suite for Drawing Glycan Structures and Assisting the Annotation of Mass Spectra

Alessio Ceroni¹, Kai Maass², Anne Dell¹, Stuart Haslam¹

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²Institute of Biochemistry, Faculty of Medicine, University of Giessen, Germany



“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 main component of “GlycoWorkbench” is the visual editor for glycan structures. Using the editor, multiple structures can be assembled and displayed at the same time. The residues are displayed using a symbolic representation for monosaccharides, and their graphical placement is automatically carried out following appropriate rules. Various symbolic notations can be employed, such as the CFG notation (1), a 2D textual representation and the notation adopted by prof. Rudd’s group (2). All the structural features such as residue conformation, linkage position, substitutions and reducing end markers can be specified and displayed. Additionally, the structures can be exported to file in common graphical formats or copied as figures into the most popular document editors. The editor will soon be able to import and export structures in the GlycoCT format. A version of the editor that can be integrated into web pages will also be released. This web editor will be used wherever a structure is requested as input or needs to be displayed from its string encoding.

“GlycoWorkbench” has been designed to assist the process of structure determination from MS data by automating the repetitive tasks carried out during the interpretation of experimental results. While the structure is being drawn the monoisotopic and/or average mass are automatically computed and displayed, either for the underivatized, peracetylated or permethylated glycan. After a structure is built, all its possible fragments (multiple glycosidic cleavages {B/C/Y/Z}, cross-ring cleavages {A/X} and their combinations) can be computed and shown with their associated masses

(similarly to “Glyco-Fragment” (3)). The list of fragments from one or multiple structure can then be matched to a list of peaks imported from file. The results of the peak list matching are shown in several reports to highlight different aspect of the proposed annotation: one table shows for each structure the peak list annotated with its fragments; another report shows the annotations (fragments) from all models for each peak; finally, a statistics table displays for each structure several measures of the quantity of annotated peaks, to have a comparison of the models’ quality.

To add flexibility to “GlycoWorkbench” an integration with the “Glyco-Peakfinder” (4) tool is planned. “Glyco-Peakfinder” estimates the composition of a glycan from MSn data and produce a structural model by matching the composition with a database of structures. When the “GlycoWorkbench” will be able to import structure from GlycoCT files, the automatically derived structures could then be loaded into the editor, refined and modified by the user, matched against the peak list and compared according to the various available statistics to decide the best candidate.

The latest version of “GlycoWorkbench” and the user manual can be retrieved from:

<http://www.eurocarbodb.org/applications/ms-tools>

[1] www.functionalglycomics.org

[2] L. Royle, R.A. Dwek and P.M. Rudd, in Current Protocols in Protein Science, John Wiley & Sons, 2006

[3] K.K. Lohmann and C.-W. von der Lieth, Nucleic Acid Research, 32 (Web Server Issue): W261-W266, 2004.

[4] “Glyco-Peakfinder” is presented on another contribution.

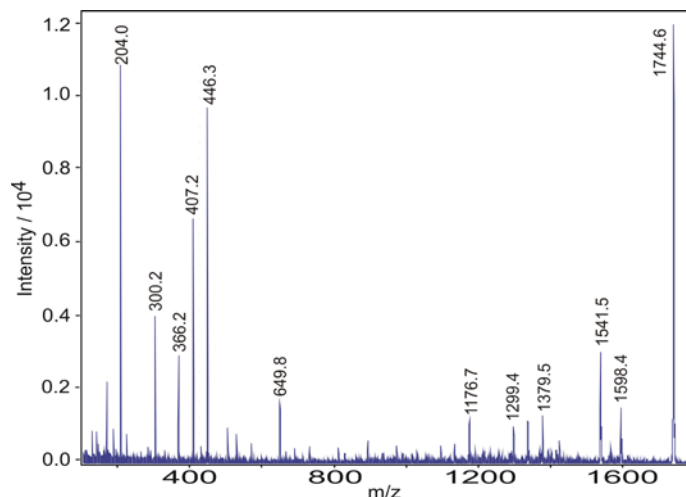
GlycoPeakfinder

Automated Annotation for MS Peaks of Carbohydrates

Kai Maass¹, René Ranzinger², Hildegard Geyer¹, Claus-W. von der Lieth² and Rudolf Geyer¹

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Automatic processing of mass spectrometric data in the field of glycomics is still an evolving field when compared to the field of proteomics. Up to now, neither large structural databases nor software tools are available which provide a complete workflow from experimental data to glycan structure determination.

The “Glyco-Peakfinder” is a web-based software application for fast and automated annotation of peaks of all kinds of mass spectra of glycans. All possible compositions for a peak from a given mass list, using a strategy comparable to composition-based sequencing developed for peptides (1) can be calculated.

“Glyco-Peakfinder” can be used both for analysis of sample profiling and for identification of fragments in MSn spectra, as different series of ions, such as, A-, B-, C-, X-, Y- and Z- ions can be calculated in parallel. The option of detecting differently- and/or multiply-charged ions in one calculation cycle enables 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 –, consideration of non-carbohydrate moieties or identification of glycopeptides with known peptide sequences) increase the field of application from native glycans to a variable set of glycoconjugates.

In addition, the results from “Glyco-Peakfinder” can be used for advanced database search in glycosciences.de (2) to assist in structure identification. A combined search with compositions of different mass peaks obtained from the same compound can be carried out. This strategy leads to an enormous decrease of structure suggestions from the database.

Finally, the results derived from calculation and the structures obtained from the database search can be exported to other software suites, such as, “GlycoWorkbench” which allows further processing, evaluation and presentation of the experimental data.

The “Glyco-Peakfinder” is available at:

<http://www.eurocarbodb.org/applications/ms-tools>

- (1) B. Spengler. (2004). *J. Am. Soc. Mass Spectrom.* 15, 703-714.
- (2) T. Lütteke, A. Bohne-Lang, A. Loss, T. Götz, M. Frank & C.-W. von der Lieth. (2006). *Glycobiology* 16, 71R-81R.
- (3) G. Lochnit, R. Geyer, *Eur. J. Biochem.*, 228, 1995, 805-818

Glyco-Peakfinder						
introduction		results	structures	fragments	settings	contact
Mass	Intensity	Composition (check for fragment and structure search)	Charged ions	Ion type	Mass calculated	Deviation [ppm]
204.000	n/a	<input type="checkbox"/> HexNac1	H+	B	204.08665	424.7
300.200	n/a	<input type="checkbox"/> HexNac1-PA	H+	Y	300.15540	-148.6
366.200	n/a	<input type="checkbox"/> Hex1HexNac1	H+	B	366.13947	-165.3
407.200	n/a	<input type="checkbox"/> HexNac2	H+	B	407.16602	-83.4
446.300	n/a	<input type="checkbox"/> HexNac1dHex1-PA	H+	Y	446.21331	-194.3
1176.700	n/a	<input type="checkbox"/> Hex6HexNac1	H+	B	1176.40359	-251.9
		<input type="checkbox"/> Hex2HexNac3dHex1-PA	H+	Y	1176.47770	-188.9
		<input type="checkbox"/> HexNac2dHex2NeuAc2	H+	C	1299.48323	-166.8
1299.700	n/a	<input type="checkbox"/> Hex7dHex1	H+	C	1299.44551	-195.8
		<input type="checkbox"/> Hex3HexNac4	H+	B	1299.48323	-166.8
		<input type="checkbox"/> Hex3dHex2NeuAc2	H+	C	1379.48296	-12.4
1379.500	n/a	<input type="checkbox"/> Hex6HexNac2	H+	B	1379.48296	-12.4
		<input type="checkbox"/> Hex2HexNac4dHex1-PA	H+	Y	1379.55707	41.4
		<input type="checkbox"/> Hex4dHex2NeuAc2	H+	C	1541.53578	23.2
1541.500	n/a	<input type="checkbox"/> HexNac4dHex1NeuAc2	H+	B	1541.57350	47.7
		<input type="checkbox"/> Hex7HexNac2	H+	B	1541.53578	23.2
		<input type="checkbox"/> Hex3HexNac4dHex1-PA	H+	Y	1541.60989	71.3
1744.700	n/a	<input type="checkbox"/> Hex4HexNac1dHex2NeuAc2	H+	C	1744.61515	-48.6
		<input type="checkbox"/> HexNac5dHex1NeuAc2	H+	B	1744.65288	-27.0
		<input type="checkbox"/> Hex7HexNac3	H+	B	1744.61515	-48.6
		<input checked="" type="checkbox"/> Hex3HexNac5dHex1-PA	H+	Y	1744.68926	-6.2

Result of composition search for peaklist from a pyridylamino-oligosaccharide fraction obtained from batroxobin of *Bothrops moojeni* venom (3)

European-Japanese Glycomics Workshop

A two day workshop in glycomics was held in September 2005 in Florence, Italy. The topics of the presentations covered analytical, functional and medical aspects of carbohydrates as well as bioinformatics. Especially young scientists were encouraged to present their work in short presentations to an audience containing leading experts in the field.

The workshop was organized by the Human Disease Glycomics/Proteome Initiative (www.hgpi.jp) in collaboration with the EUROCarbDB consortium.



Program of the European-Japanese Glycomics Workshop
supported by the core to core program (www.jpss.go.jp/english/core_to_core) Japan Society for the Promotion of Science (JSPS) and EuroCarbDB-project (www.eurocarb.org).

Florence September 3rd and 4th

Saturday, September 3rd

12:30-13:00 Registration
13:00-13:15 Welcome and Introduction
Chair Kunihiko Suzuki
13:15-13:30 Rita Gerardy-Schahn, Hanno
Phenotype characteristic of
synthetase
13:30-13:45 Kazuyuki Nakamura, Yamag
Sialylated apolipoprotein E in
13:45-14:00 Rüdiger Horstkorte, Berlin G
Polysialylierung and Bioche



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Impressum

EUROCarbDB Newsletter (01.11.2006)

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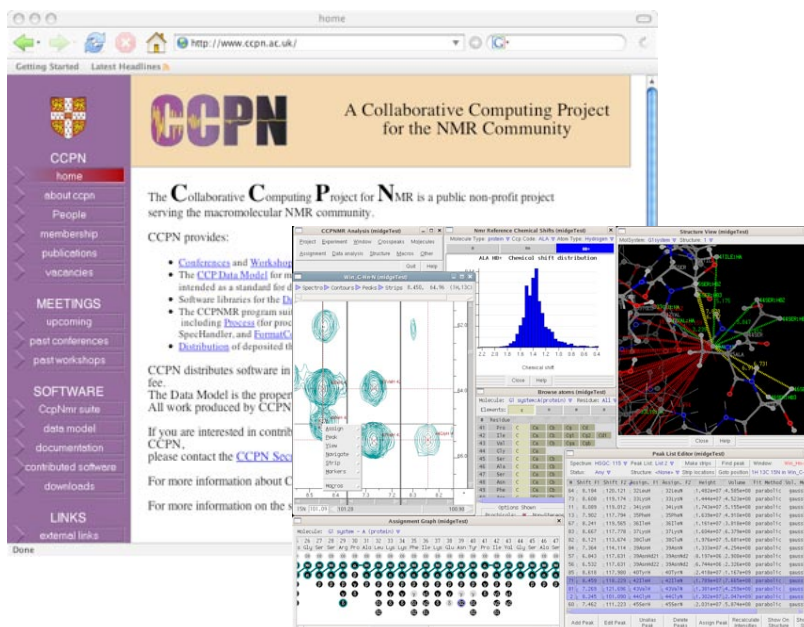
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The screenshot shows the CCPN website with the title "A Collaborative Computing Project for the NMR Community". It lists various software tools and data models provided by CCPN, such as the CCP Data Model, software libraries for data processing, and the CCPNMR program suite. The interface also displays several NMR spectra and chemical structures.

In EUROCarbDB DS4 (NMR) we have recently started a new collaboration with CCPN (www.ccpn.ac.uk). Initial work has been done to generate ChemComp XML of carbohydrates (see also www.ebi.ac.uk/msd-srv/docs/NMR/main.html). The project will be described in more detail in the next EUROCarbDB newsletter.