

Computational platforms for large-scale proteomics

Proteomics software producer GeneBio SA and Genedata AG, a provider of computational solutions for drug discovery and development, are collaborating on high-throughput solutions for analysing proteomics data for drug discovery.

Swiss company Geneva Bioinformatics (GeneBio) SA offers original educational and knowledge-discovery solutions that help scientists convert a range of information into biological knowledge. The company was founded in 1997 in parallel with the establishment of the Swiss Institute of Bioinformatics (SIB). The company has evolved from its initial mandate of commercialising databases and other products developed by the SIB into a global multifaceted bioinformatics company offering a broad range of original solutions.

Challenges in bioinformatics

"Life sciences have been continuously revolutionised in the rate of data accumulation and in the diversity of the biological information being generated through a multitude of technologies," says GeneBio's CEO, Nasri Nahas. "The industry has dramatically changed over the past 20 years; and we are now more in a 'knowledge-limited' rather than 'information-limited' era. The industry is now confronted with the ever-growing problem of transforming these masses of heterogeneous information into integrated and structured knowledge.

"While the bioinformatics industry has undergone significant growth in the past, the challenge for tomorrow's bioinformatics remains. If this industry desires to continue maturing and playing a central role in modern life sciences, it must rise to the challenge by providing tools to generate easily understandable synthetic views that take into account different types and natures of information; being modular and flexible enough in order to accommodate constant and evolving adaptation of life science knowledge; and positioning itself as a facilitator, rather than a replacement, of human decision. Human expertise will



Pictured are Pierre-Alain Binz and Anne Niknejad, members of GeneBio's Phenyx Team. Phenyx is one of the company's products, a software platform for the identification and characterisation of proteins and peptides from mass spectrometry data; Binz is the product manager for Phenyx, and Niknejad is the senior product specialist.

always remain the ultimate reference: bioinformatics tools should focus on adding value to the existing human element instead of trying to completely replace it.

"The challenge today is to overcome the information bottleneck by putting together the right information in a contextualised manner in order to allow research scientists to corroborate those separate pieces of information, and thus to generate pertinent biological knowledge," he says.

To enable its customers to bridge the gap between information gathering and knowledge generation, GeneBio offers products and services developed through its own expertise as well as by promoting specific valuable products developed by renowned academic institutions and commercial companies. The company's offerings include software platforms, training services and content solutions.

Protein identification and characterisation

GeneBio retains close ties to the company's academic peers, allowing its development teams access to researchers in order to realise solutions to complex problems. The software platforms developed can be used as stand-alone products or incorporated into broader solutions in specialist applications. The company maintains a network of strategic partnerships that allow it to incorporate external concepts and technologies as intrinsic elements of its platforms and, likewise, to integrate its technologies into third parties' platforms, giving it the flexibility to work efficiently within a very broad range of complex systems. Its expertise is in a variety of proteomics applications, with major emphases on protein identification and characterisation, as well as in proteome imaging.

The company's collaborations with research institutes, notably the SIB, for novel solutions for the proteomics market, have a special focus on mass spectrometry-based techniques. One example of this focus is the creation of Phenyx, a next-generation protein characterisation platform developed while working with proteomics scientists. Phenyx is specifically designed to meet the concurrent demands of high-throughput MS data analysis and dynamic results assessment.

Mass spectrometry (MS) is a powerful technology that plays a central role in a number of proteomics experimental workflows. The variability of sample preparation procedures, of available MS instrumentation and of possibilities to run the instrumentation highlights the heterogeneity of data to process and then to interpret. Bioinformatics tools are necessary to carry out peptide and protein identification, characterisation and quantitation from these data, while in addition considering the heterogeneity of quality and quantity of the data. In order to evaluate and qualify the results of these processes, the sole existence of appropriate algorithms is not sufficient. More and more end-users need to have access to a battery of qualifying and validating tools and

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GeneBio's CEO, Nasri Nahas: overcoming the information bottleneck to generate biological knowledge.

principles to extract the biological relevance of the results.

Proteome imaging

One example of GeneBio's proteome imaging focus is the collaboration the company has had with the SIB over the past several years in developing algorithms that have been incorporated into its Melanie software package, an algorithm and imaging platform for 2-D gel analysis. The software provides solutions to shorten the path from

data acquisition to protein information. Its detection system and algorithms facilitate the extraction of statistically valid differences between groups of 2-D gels, allowing users to more easily analyse and present results from 2-D gel electrophoresis experiments.

SIB proteomics databases

Since 1998, GeneBio has provided researchers with access to a number of SIB proteomics databases for research optimisation. The Swiss-Prot knowledgebase is an extensively cross-linked database that connects the various findings in the diverse field of proteomics research: PROSITE is a database of protein families and domains, based on the observation that while there are very many different proteins, most of them can be grouped on the basis of similarities in their sequences to form a limited number of protein families, the members of which generally share functional attributes; and SWISS-2DPAGE is an annotated two-dimensional polyacrylamide gel electrophoresis database established in 1993. The database provides textual data on proteins and cross-references to other databases and Swiss-Prot.

Strategic alliances

GeneBio continues to seek and establish partnerships with leading academic and commercial organisations in order to expand its external assets and further its collaborative network. The company recently established a collaboration with another



Othmar Pfannes, CTO of Genedata: empowering researchers to identify and validate biomarkers.

Swiss company, Basel-based Genedata AG, a global provider of computational solutions for drug discovery and development, to offer life science researchers a precise, high-throughput solution for analysing proteomics data.

The two companies will integrate Genedata's Expressionist solution with GeneBio's Melanie/ImageMaster 2D Platinum solution, forming a seamless analysis workflow. Expressionist automates analysis workflows from sample validation through to result management.

"There is a growing need for integrated, reproducible and scalable

methods to exploit proteomics data," explains Nahas. "The next phase in the collaboration involves incorporating Expressionist with GeneBio's Phenyx mass spectrometry (MS) data analysis platform, specifically designed to meet the concurrent demands of high-throughput MS data analysis and dynamic results assessment. This collaboration builds on synergies between our systems and delivers robust automation of proteomics analysis."

"Pharmaceutical companies are combining data from multiple technologies, including MS, in their biomarker discovery efforts," adds Dr Othmar Pfannes, CTO of Genedata AG. "The system empowers researchers to identify and validate biomarkers using different technological platforms, including high-throughput proteomics applications."

Genedata specialises in computational solutions for life science research, drug discovery, and drug development. The company combines a comprehensive, scientifically validated computational platform with expert scientific consulting services to provide tailor-made solutions for specific applications and multiple therapeutic areas. Founded in 1997 as a spin-off from Novartis, Genedata is headquartered in Basel, Switzerland and has subsidiaries and branch offices in Germany and the USA.

The company's new MS analysis development included an extensive survey of MS technologies by engineers and physicists at the company's research centre in Munich, Germany. The result is a highly automated and standardised MS data processing platform, integrated seamlessly with Expressionist's existing analysis applications for transcriptomic and gels-based proteomic data.

"It is the degree of technology integration that makes our new MS analysis applications so valuable for biomarker discovery and represents a major step in enhancing the value of Expressionist," says Pfannes.

"Together with promoting our products, these partnerships help to further our understanding of the proteomics market and the adequacy of our products within such a highly fluid environment," adds Nahas. "This deep networking strategy allows us, while focusing on our core competencies, to pass onto our clients a wealth of scientific expertise in order to provide to the market tools matched to their current needs and enriched by high-grade applied research," he says. ^{sp²}

FURTHER INFORMATION

Andrew Smith
Geneva Bioinformatics (GeneBio) SA
25 Avenue de Champel
CH-1206 Geneva
Switzerland
Tel: +41 22 702 99 00
Fax: +41 22 702 99 99
Email: andrew.smith@genebio.com
Web: www.genebio.com

Tobe Freeman
Genedata AG
Maulbeerstrasse 46
CH-4016 Basel
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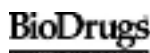
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