PEAKS® Online XPRO

ACCELERATE DISCOVERY wih

All-in-One, High-Throughput, Multi-User, Proteomics LC-MS/MS Solution

BSi

Use PEAKS Online Xpro to take advantage of powerful and shared computing resources to perform LC-MS/MS protein & peptide identification and quantification analyses. The restructured platform allows large datasets to be processed efficiently by multiple users at the same time; with the ability to run on any cluster, multi-CPU machine, or cloud server.

PEAKS is a specialized tool that embraces the complexity of a biological sample and maximizes the information uncovered for your discovery proteomics research.

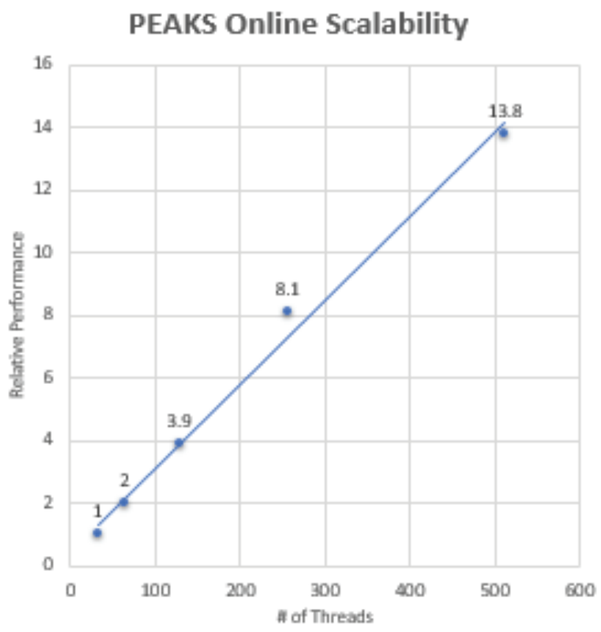
As a vendor-neutral computing platform, it is capable of directly loading raw mass spectrometry data and standard data formats. Deploy the PEAKS Xpro workflows, from de novo sequencing, PEAKS DB (database search) identification, PEAKS LIB (spectral library search), PEAKS PTM (post translational modification) analysis, and SPIDER homology search to identify the presence of peptides and proteins in your project. Quantification analysis by labeling and label-free quantification (LFQ) can also be performed using the PEAKS Q addon module. Intuitive result visualization tools are provided at every stage of analysis and results can be exported. PEAKS Online Xpro supports data-dependent and data-independent acquisition analyses (DDA and DIA respectively) and ion mobility mass spectrometry (IMS-MS).

Time	CPU Cores
17h11m	512
1 day 4h32m	256
2 days 1h24m	128
4 days 19h55m	64
9 days 15h10m	32

Data size	
# of Samples	56
Total MS runs (180 min/run)	672
MS	5,106,542
MS/MS	28,858,408

PEAKS SERVER BASED SOLUTION KEY FEATURES

Re-running analyses has never been so easy. With PEAKS Online, the algorithm will determine the quickest way to reanalyze your results and use existing results, if applicable, instead of running the whole dataset again.



Centralized configuration and monitoring system to easily maintain, prioritize and share all PEAKS Online data analyses.

Allow concurrent access from multiple users to process multiple projects in parallel.

High performance and advanced algorithms to provide a complete, vendor-neutral solution for discovery proteomics, including protein/peptide de novo sequencing, identification and quantification.

Quantification capabilities to perform label and label-free quantification (LFQ) on a large-sale level.

Don’t get left in the dark! Move Together as a Cohesive Research Group

PEAKS Online means high-throughput data processing on a shared resource. This server-designed proteomics software is fully parallelized with the ability to run on a cluster of multi-CPU machine or cloud server.

Users are able to run the same proven algorithms included in the PEAKS Studio solution, efficiently and on a larger scale.

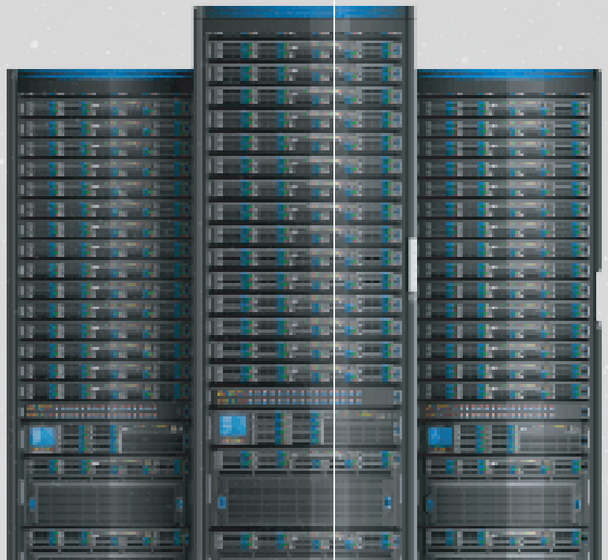
By using a web interface client, users can send/retrieve data to/from the server and view the results in an intuitive manner.

Advanced System Architecture

Built on top of latest technologies to fully utilize the computing power of your hardware to provide:

High throughput solution: Allows concurrent access from multiple users to support parallelism at project and data level.

Distributed database: Yields higher I/O performance and better fault tolerance.



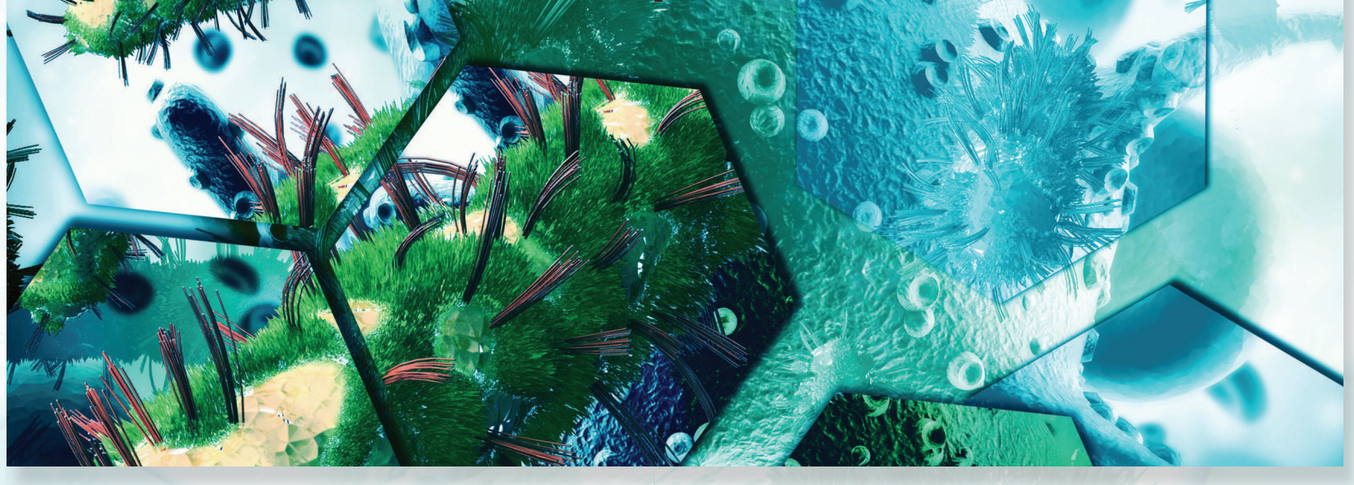
Ready to scale: Vertically and horizontally, add new worker node(s) or database node(s) to the system and see performance improvement right away.

Cross-platform deployment:
Ready to deploy on any Windows or Linux systems.

Dual interfaces: The command line interface offers the abilty to automate dtaa analysis workflows and result exporting while the web interface provides a graphical user interface to visually configure workflows and easily assess results in detail.

PEAKS' de novo peptide sequencing is well-recognized worldwide and the base of all PEAKS analyses

The innovative PEAKS' de novo sequencing algorithm accurately construct a peptide sequence without the use of a database. These sequences are then used to enhance the PEAKS DB, PEAKS PTM, and SPIDER analyses.



PEAKS enhances the separation of true/false hits by integrating de novo sequencing into a database search workflow. This unique approach identifies more peptides and proteins with increased confidence.

Examine accuracy at the amino acid level

Local confidence scores are assigned for each amino acid. You can easily separate confident amino acid assignments from false positives.

Find novel peptides not recorded in protein database

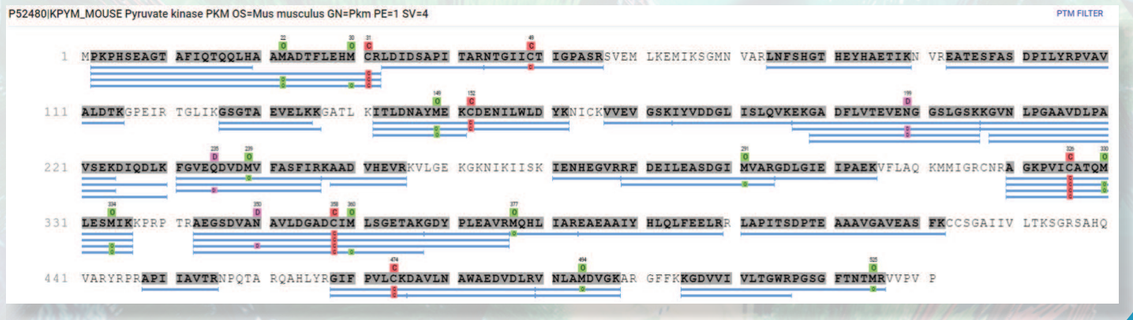
De novo results from scans missed in protein databases are summarized in 'de novo only' results. Partial protein matches or "de novo tags" are also given and can be viewed directly.

Protein coverage heatmap for quick and easy comparison across multiple samples

Easily compare between multiple samples in a project using the PEAKS Online protein coverage heatmap. The increasing colour intensity indicates a higher abundance of supporting spectra within the corresponding sample.

No need to sacrifice details when analyzing large datasets

Interested in the protein coverage in a particular sample? PEAKS Online X allows users to select an individual sample to view the detailed coverage information, just as in PEAKS Studio.



Spectral Library Search

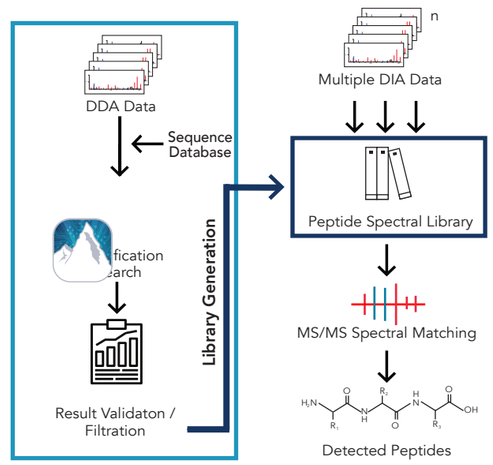
Use PEAKS Online for high-throughput analysis of large sample cohort proteomics studies to overcome the increased search space and long processing times. With the addition of the spectral library workflow researchers can focus on the purpose of the study by gathering targeted information and screen samples for known peptides and proteins.

Advantages of PEAKS Spectral Library Search

- High-throughput, scalable platform for large-scale proteomics research projects
- Screening samples for known peptides/proteins
- Improved sensitivity for single cell proteomics and other low abundant data

One package to take you from start to finish

Given a spectrum and spectral library, find a peptide in the spectral library that has the best match with the spectrum



1 Create a database library with DDA data to analyze with DIA data. The library you have generated can by used multiple times with DIA data.

2 Peptide Spectral Library will compare peptides from the new library search dataset to the dataset generated.

Creating a library is as simple as one click

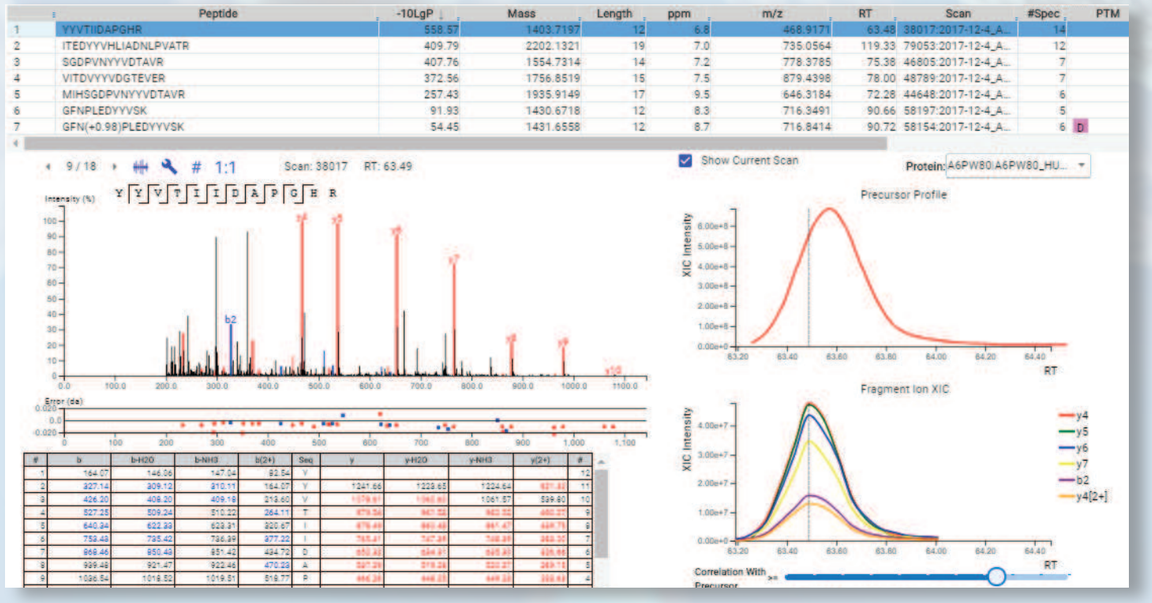
Easily generate a spectral library with PEAKS Online by simply selecting the desired PEAKS identification results from your list of completed analyses. Alternatively, PEAKS Online supports library generation from external sources.

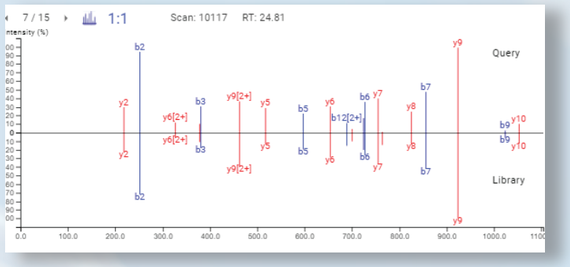
Establish standardized data anaylsis workflows

For Biopharma and CRO companies it is important to operate with standardized workflows to maintain compliance and streamline the data analysis processes. Extend your Standard Operating Protocols (SOPs), from your wet lab to your data analysis by creating set workflows in PEAKS Online for future repeated use.

Spectral library workflows are commonly used for DIA data analysis to exploit the technology behind DIA data without the hassle of long processing times.

Increased complexity of DIA data is a result of its information-rich acquisition method. DIA data provides highly accurate information on MS1 and MS2 levels with few missing values. Precursor Profile and Fragment Ion XIC views have been added to help with quality control and validation.





Click the icon to view the Query vs. Library Mirror Plot. Using a spectral library, you can match the observed spectra to the identified spectra.

PEAKS Online presents an intuitive GUI to allow results to be examined at all levels of the data. Fully interrogate the data from the spectra-, to the peptide-, to the protein-level for comprehensive understanding of the spectral library search results.

Addition of a sequence database with your spectral library allows protein inference. Easily determine the source of your peptide using the protein coverage view and compaare how they vary from one sample to the next

Designed to discover hidden modifications

In PEAKS PTM, the unassigned spectra with highly confident de novo scores are reanalyzed to assess any unknown or unexpected modifications. Use a set list of your PTMs of interest, or turn on all 313 naturally occurring, biological modifications from the Unimod database. This multiple-round search approach can help you maximize the identification and sensitivity of your PTM analysis.

Site localization confidence and result validation

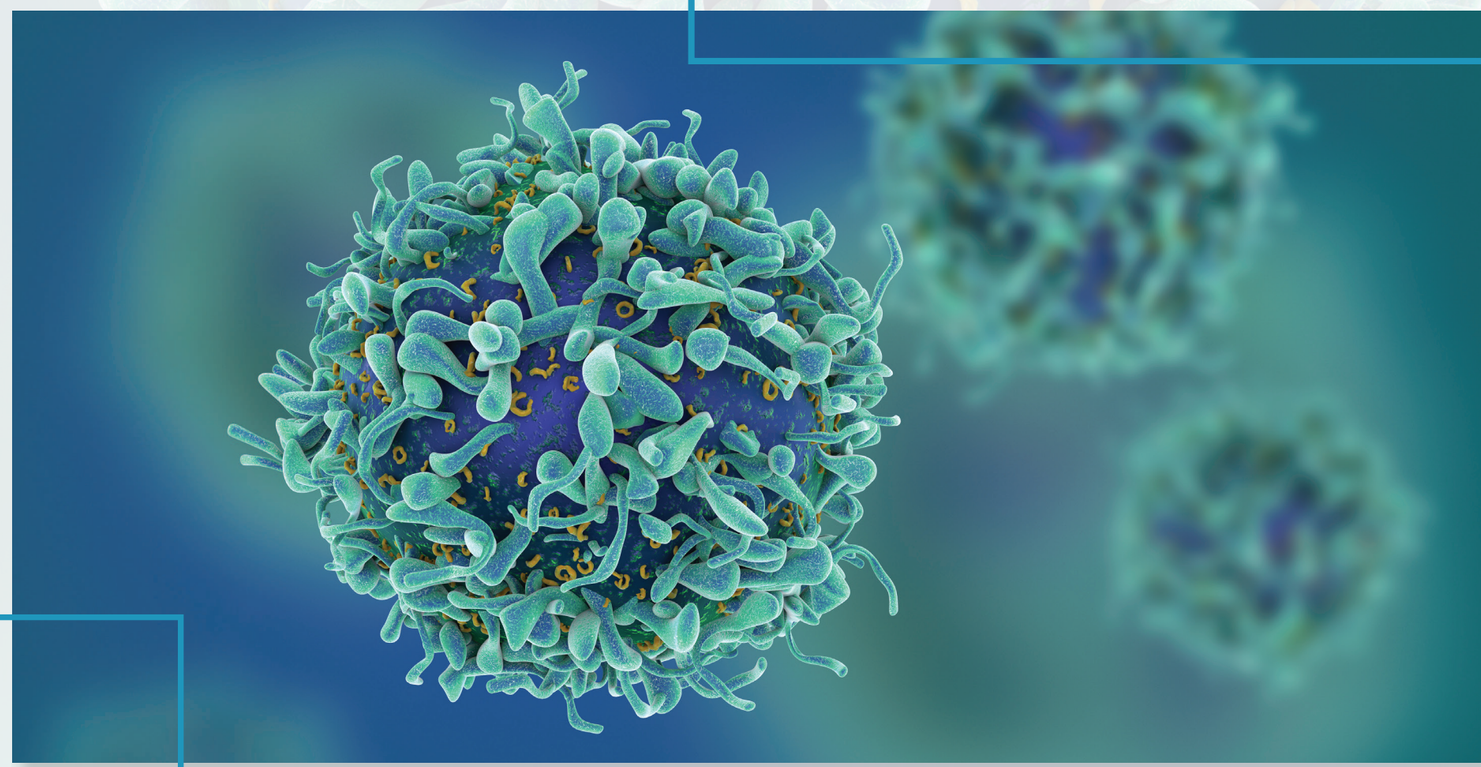
Use PEAKS to measure the probability of any given local site modifications by assessing it's A-Score and/or ion intensity. Allow PEAKS to help you confidently report identified PTMs and sequence variants.

Cross-species homology search with SPIDER

De novo tag homology search tolerates common de novo sequencing errors such as (AT/TA) and (N/GG). Find confident hits that are different from the database entry with our de novo tailored homology search.

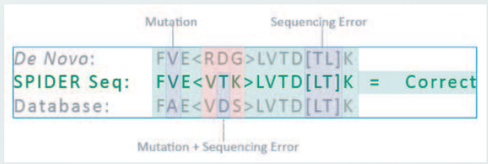
SPIDER provides a specialized approach for:

- Resolving database errors
- Antibody sequence confirmation
- Potential biomarker discovery
- Mutated peptide identification



Powered by de novo sequencing to reconstruct the true sequence

SPIDER tries to match the de novo sequence tags with the database proteins. By minimizing the sum of the de novo errors between the reference sequence and the de novo sequence, SPIDER, reconstructs a "real" sequence to find peptides with single amino acid variants.



The characterization of PTMs and sequence variants is crucial to the understanding of biological pathways.

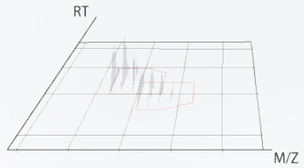
Add the PEAKS Q module to your PEAKS Online data analysis workflow for robust label & label-free quantification

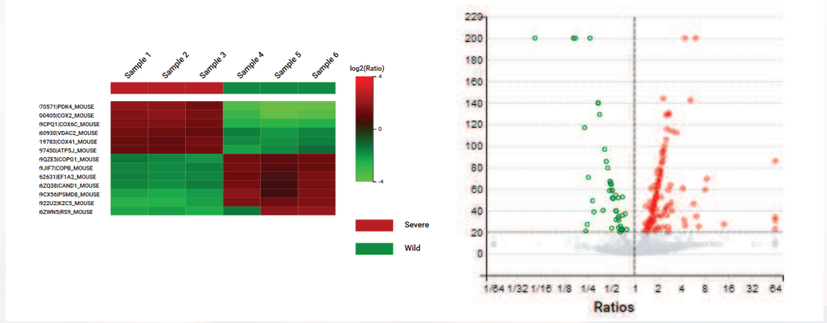
Accurate and sensitive protein- and peptide-level quantification in all dimensions

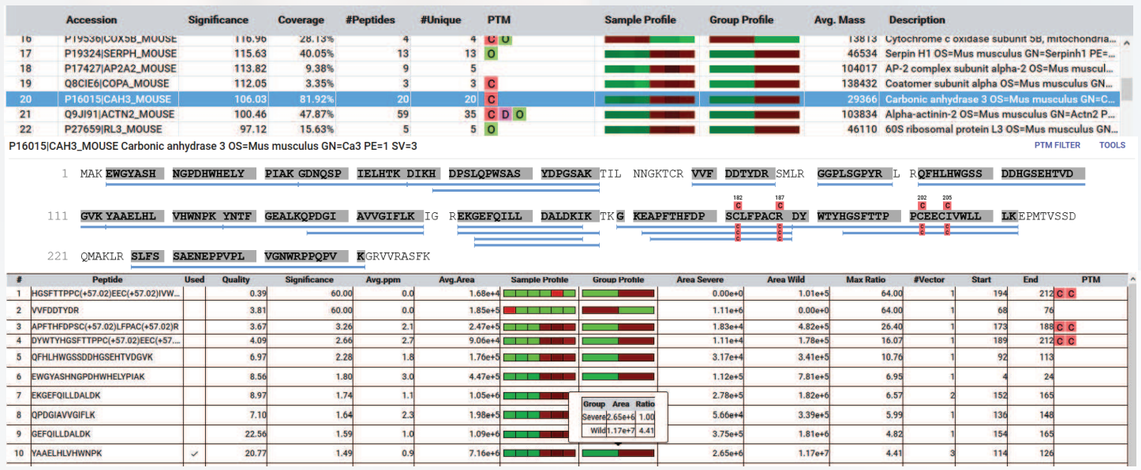
To achieve accurate and sensitive quantification for the large amount of data collected from LFQ experiments, use PEAKS Q to automate ion peak alignment and comparison. Users with access to IMS-MS technology for the extra 4th- ion mobility dimension, enable the PEAKS IMS module to further enhance feature alignment for more accurate quantification results.

Easily interpret protein and peptide change in abundance between samples and groups

PEAKS Q presents its quantitative results in various graphs and charts to quickly analyze the change in proteins and peptides with just a glance at the results. Export the results in text format for precise, detailed information.







Priority processing for multi-user platform

Ensure deadlines are met by assigning priority to the analyses. Default priority can be set per user, and priority can be adjusted once an analysis has begun. Users can also receive an email notification when analysis is complete.

Developed to align your team's efforts

With PEAKS Online, the administrator(s) has centralized control to allow the standardization of workflows, parameters, and databases from one data analysis to the next.

Work as team and collaborate with ease

In PEAKS Online, users can easily share projects, databases, workflows, and even parameters between the whole research team.

Easily monitor performance of PEAKS Online

Administrator(s) of PEAKS Online can check the usage of the master and worker nodes to make sure everything is running at optimal performance.

Bioinformatics Solutions Inc.
470 Weber Street North, Suite 204
Waterloo, Ontario N2L 6J2
Canada
Tel: (519) 885-8288
Fax: (519) 885-9075
sales@bioinfor.com
www.bioinfor.com