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BioNumerics SEVEN

Applied Maths proudly presents BioNumerics version 7.5, honoring a good old Applied Maths tradition of supplying its "minor" upgrade with a new features list worth the label "major". The main new features of this v7.5 release include the redesigned MLVA plugin, the calculation engine providing computing power in the cloud and the brand-new whole genome MLST plugin. Attention has also been given to further enhancement of the software's performance and storage possibilities, as well as easily operated export functions. Furthermore, we now offer the opportunity to analyze subsets of experimental data for character, fingerprint and spectrum experiment types, linked to the entries in a comparison. If your interest is sparked, please see below for a more elaborate overview of the innovations for this notable upgrade.

NEW FEATURES IN BIONUMERICS v7.5

GENERAL FUNCTIONALITY

- The software now runs natively on 64-bit Windows, greatly improving speed and performance.
- New embedded file-based SQLite database engine, for hassle-free setup of large (up to 32TB!) databases.
- Easy data migration from MS Access connected databases to more professional databases avoids issues with Access' 2GB storage limit.
- New preview options in most import routines allow a quick inspection of import templates and data parsing.
- Recently used import routines are conveniently grouped together for easy access.
- Vastly enhanced export options for graphical content. Direct export to TIFF, PNG, PDF, SVG, etc. files is now possible.
- Easier and more flexible data exchange between BioNumerics databases.
- The *Processing wizard*, a new one-click tool has been developed to quickly initiate common or routine operations on selected entries.
- "Don't show this message again" logic avoids the display of superfluous confirmation messages.
- Back by popular demand: bring selected entries to top functionality (keyboard shortcut Ctrl+T).

FINGERPRINT ANALYSIS

GEL IMAGE EDITOR

- Improved handling of 12-bit TIFF gel images.

BAND CLASSES

- New *band class views* offer an easy tool to perform cluster analyses and statistical tests on predefined subsets of band classes.
- Custom fields are available for storage of band class metadata.

CAPILLARY SEQUENCER DATA IMPORT AND ANALYSIS

- More flexible import of electropherograms generated by capillary sequencers.
- Improved band search with separate settings for reference channels (containing the size markers) and data channels.
- Easier band selection in the *Curve processing window* for manual edits.

CHARACTERS

- New *character views* allow the user to switch easily between predefined subsets of characters.
- A mapping cost matrix for specifying biologically relevant similarities when clustering categorical character types based on their mapping.

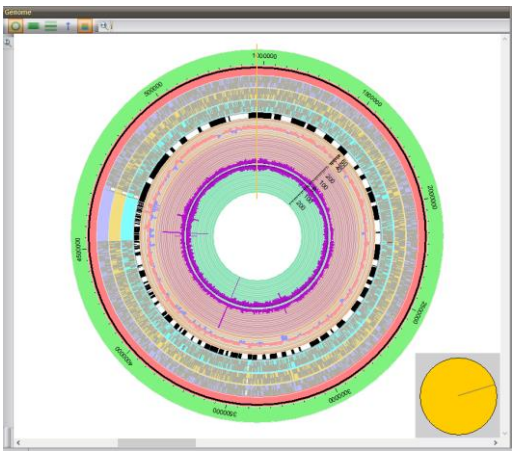
SEQUENCE ANALYSIS

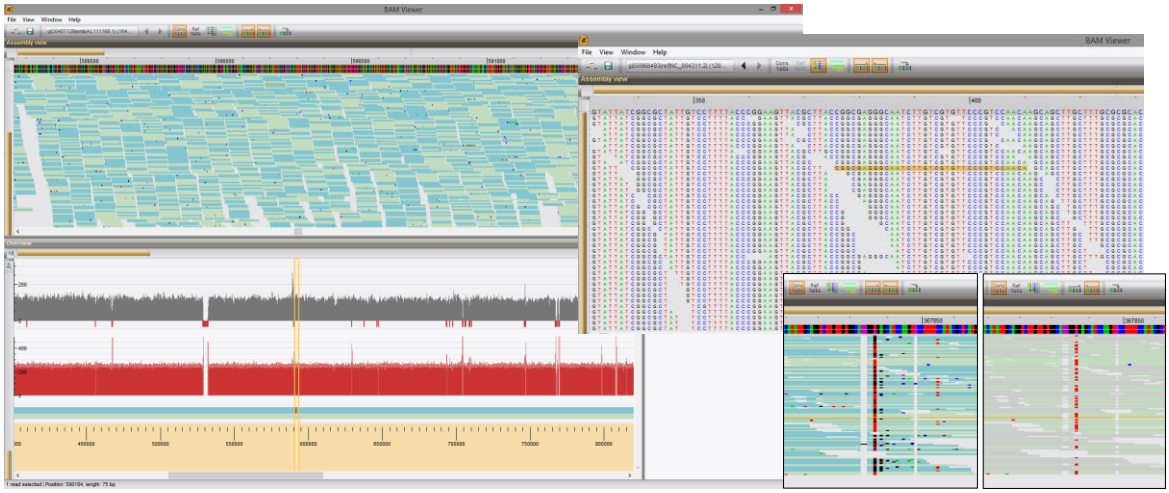
SANGER SEQUENCING

- More flexible import and batch assembly of sequencer trace files.
- Existing assemblies can be re-trimmed and/or reassembled without reimporting the trace files.
- Files in FASTA format can be imported and assembled in the BioNumerics *Assembler*.

NEXT GENERATION SEQUENCING

- When using a known reference sequence to assist the assembly, the new *Map to reference* algorithm, maps reads to a reference sequence with respect to the position in the reference sequence. This is highly valuable for SNP analysis.
- Flexible display of genomic sequences, with multiple channels and custom curves in the new *circular genome viewer*.
- The new SAM/BAM file import allows the user to take advantage of BioNumerics' post-processing capabilities for existing sequence assemblies.





TREND DATA

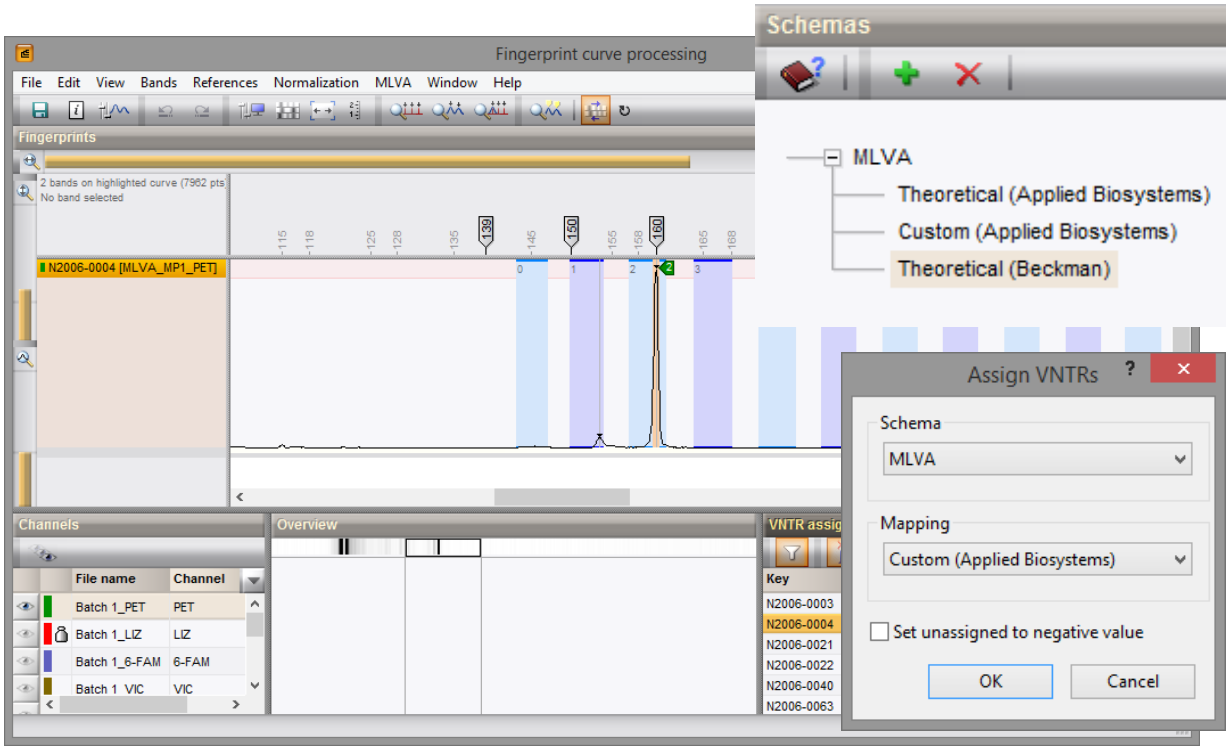
- Import of phenotypic micro-array data from Biolog's Omnilog instrument is made possible.

PLUGINS

MLVA PLUGIN

The MLVA plugin has received a substantial revision in BioNumerics 7.5:

- Seamless integration with the *Fingerprint curve processing window*.
- Multiple MLVA schemas can be used per database, which is especially useful for databases containing information about more than one bacterial species.
- A new *MLVA management window* to conveniently manage MLVA schemas, VNTR definitions and mappings.
- Easy click-and-drag editing of the VNTR bins in custom mappings.
- New options to import/export MLVA schemas and VNTR mappings, facilitating peer-to-peer data exchange.
- For labs using capillary electrophoresis equipment from different vendors, multiple instrument types can be defined and associated with an MLVA schema.
- Tools for MLVA typing, i.e. assigning VNTR marker repeat combinations to "MLVA types", similar to the procedure used in MLST, are provided.
- When double VNTR alleles are observed, the new plugin can now handle double VNTR assignments via *character mapping similarity matrices.*

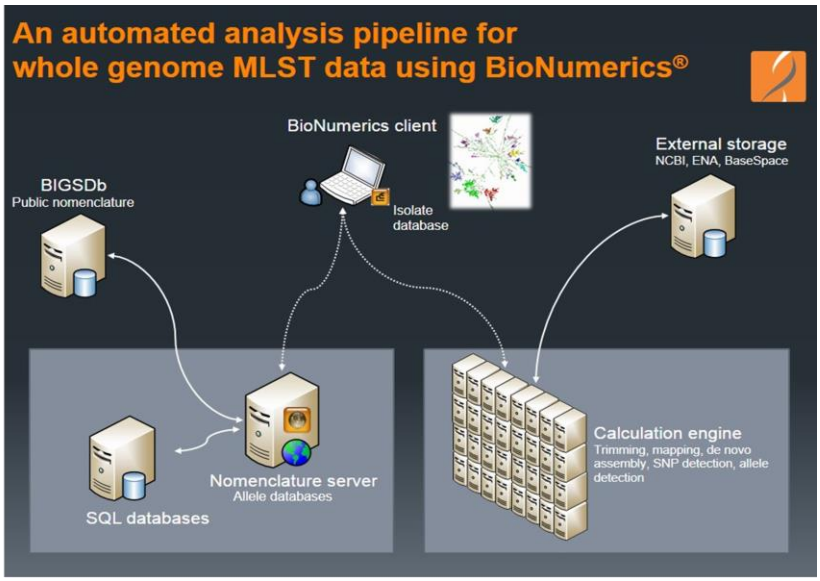


RDP PLUGIN

- Direct and easy querying of the online Ribosomal Database Project (RDP) for taxonomic identifications of strains based on their 16S rDNA sequences.

WHOLE GENOME MLST PLUGIN

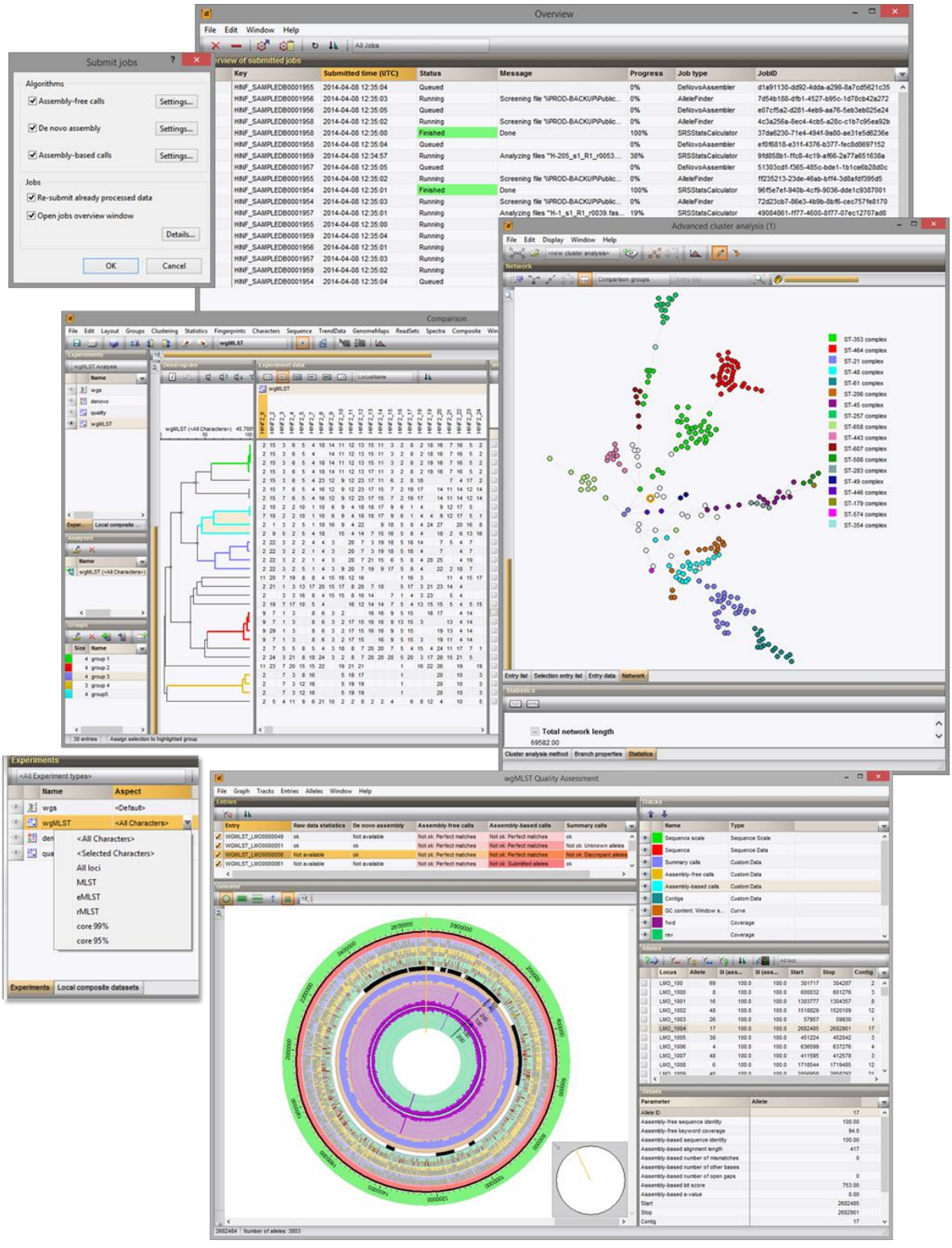
As next-generation sequencing is increasingly replacing Sanger sequencing, conventional MLST is gradually extending to whole genome MLST (wgMLST), providing higher resolution. Given the amount of data and the demanding calculations, we developed an automated pipeline with an integrated calculation engine and external storage, so it remains workable from a good average client computer.



Demanding calculations such as de novo assemblies can be performed on an external calculation engine. The choice here is offered between virtually setup-free pay-per-use cloud solutions (e.g. via Amazon) or a local deployment e.g. on a computer cluster (requires custom services). Only the wgMLST allelic profiles are stored in the BioNumerics database, resulting in a lightweight and responsive strain database.

- Import of sequence read sets from various sequencers (Roche 454®, Illumina®, PacBio®, IonTorrent®) and different sources (NCBI, EMBL-EBI, Illumina® Basespace® or Amazon S3). Sequence read sets can be imported as links to these online databases, bypassing the tedious step of up- and downloading the files.
- Batch job processing on the calculation engine to calculate read statistics, perform de novo assemblies, detect loci presence and perform allele identifications using both assembly-based and assembly-free methods.
- Overview and management of the submitted jobs with details on users, submission time, job status and progress is accessible through the Overview window. Double-click on a job displays the job log information.
- The import of job results in the database once processing is finished and automated linkage to the corresponding entry information
- Quality assessment of the wgMLST results, including imperfect and new allele matches, multiple allele matches or non-consensus allele calls.
- Automated submission of new alleles to the allele nomenclature server.
- Synchronization between the wgMLST sample database and the wgMLST typing schemes defined at server side.
- Automated assignments of sequence type and clonal complex information.

- Flexible sample reporting for the different wgMLST subtyping schemes defined in the database.
- Calculate population modelling networks in the finest and most comprehensive cluster analysis application available today, using standard or custom priority rules and with branch significance support indication.
- Calculate and display partitioning for clonal complexes and use BioNumerics' rich set of statistics tools.



CLUSTERING AND COMPARISON

- Subsets of characters, peak classes and band classes (= *aspects*) can be visualized and used in various follow-up analyses.
- An extra drop-down list in the toolbar for the character experiment type allows the user to select a field for the character labels.
- Possibility to create on-the-fly *local* composite data sets directly within the *Comparison window*, speeding up the composite analysis workflow.
- Spectrum peak class types have been replaced with spectrum peak class views.
- Now possible to add a legend for assigned comparison groups, with names and colors.
- Vastly enhanced export options for dendrograms and other graphical content. Direct export to TIFF, PNG, PDF, SVG, etc. files is now possible.
- The layout of the print preview window can be saved as a template for repeated use.

ABOUT THE BIONUMERICS PROGRAM

The BioNumerics platform is a modular software environment for the integrated analysis of all your biological data. BioNumerics can be configured exactly to match your research needs!

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