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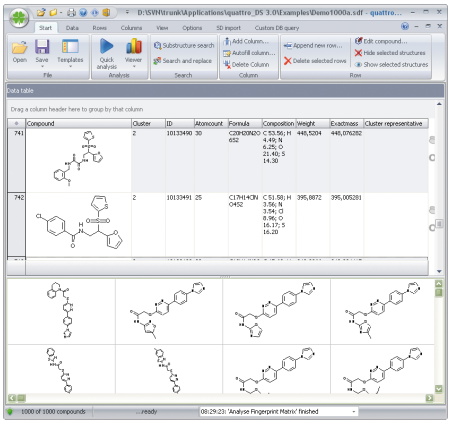
quattro/DS – Chemical Spreadsheet

Is your business drug development with small molecules? Do you need to identify drug candidates from large collections of compound libraries? Do you need to analyze and visualize your data from High Throughput Screening (HTS) and Virtual High Throughput Screening (vHTS) experiments?

quattro/DS will support your process of lead identification and optimization.

Key Features



- Handy spreadsheet-like user interface
- Advanced chemical structure support
- Easy SD files handling:
  - copy, paste and calculation functions
  - split and merge SD files
  - find duplicates
- Highly optimized numerical algorithms: processing of large molecule sets (more than 30,000 molecules) in nearly real-time
- Detection of hidden correlations between datasets by multi-dimensional statistics and cluster-algorithms
- Extensive data visualization and filtering functionalities
- Sorting and grouping of data
- Chemical structure support:
  - handling and visualization of chemical structures
  - searching within the spreadsheets: searching the data by substructure or by Tanimoto similarity
- Calculation of molecular properties, e.g. stereo configuration, SMILES, molecular weight etc.
- Customizable user interface: SDF grid, interactive charts and filters can be customized by the user. Layout templates can be defined and easily shared among user groups.
- Oracle interface, query builder
- Export filters supporting Microsoft Excel®, HTML, XML, SDF and RTF

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quattro/DS - What are your benefits?

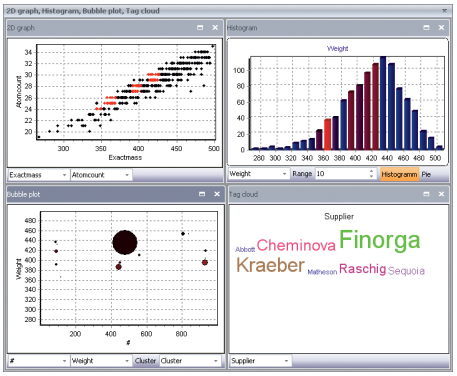
Multivariate Analysis, Visualization and Data Filtering

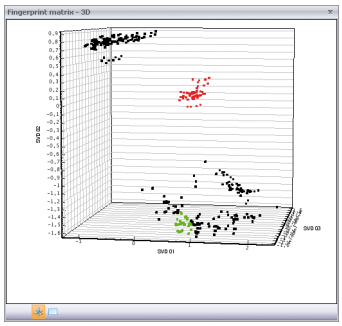
You need a powerful tool for the analysis and visualization of your HTS and vHTS data due to their multidimensional character.

quattro/DS utilizes methods of the multivariate statistics to provide you an insight into the structures of your compound data sets. Your data are visualized in a variety of interactive charts like 2D/3D scatter plots, histograms, bubble plots etc.

These charts can be used to filter the SDF data in real time: filters, e.g. based on chemical structure, can be added to find exactly the data needed. Interactive filter sliders help to optimize the amount of data filtered.

Compound groups within the charts can be selected. The selected compounds are color-highlighted in the spreadsheet and can be further processed or exported for additional analysis.





Clustering

During lead optimization, it has to be decided which candidates should continue running through the drug discovery process.

quattro/DS can support your decision with its integrated cluster algorithms. These cluster algorithms are based on chemical fingerprints and allow clustering of the data sets. Clusters are shown both in interactive graphs and in grids which can be used to select either a whole cluster or a representative.

All compounds of the data set are classified into cluster groups, and representative compounds are determined automatically.

Additional Features

quattro/DS has many more features for advanced data analysis:

- Histogram calculations for numeric and textual data
- Calculation of data by means of mathematical expressions
- Integration of standard applications for chemical structure editing like Isis/Draw® or Chemdraw®
- Color-highlighting as a result of numerical values (e.g. vHTS scores)

Contact

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Download a 60-day
quattro/DS demo version
from our website!