

ViSoR Virtual Screening optimizing the Reality – Added value from virtual and assay-based screening

With the browser based IT platform ViSoR (Virtual Screening optimizing the Reality), c.a.r.u.s. is offering a highly innovative and worldwide unique workplace for knowledge management within the context of pharmaceutical drug development.

Integration of chemical knowledge

ViSoR's key to success is based on the intelligent integration of *in vitro* and *in silico* methods within the ViSoR database. The combination of the results from virtual and assay based screening into a single environment that understands the language of the chemist results in considerable additional benefits for the scientist and better research results in a shorter time.

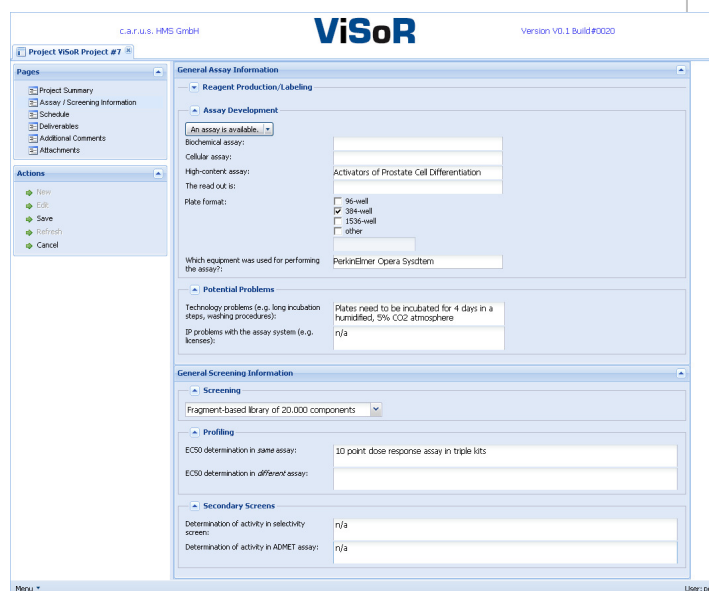
ViSoR always considers chemical compounds with all their associated properties. The calculation of the relevant physical and chemical parameters is carried out during the computation of the similarity analyses. Data files from the corresponding visualisation of 2D and 3D structures can be converted into all common file formats for export. The open architecture permits simple linking of external databases and tools and thus leaves the scientist free to concentrate on his day-to-day work.

Competent partner

ViSoR stands out because of a thorough integration of virtual screening methods. c.a.r.u.s. supports the Center for Bioinformatics of the University of Hamburg in the development of the virtual screening software TrixX. TrixX uses a special index for virtual screening and enables the identification of hits in sublinear runtime.



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The screenshot shows the ViSoR web application interface. The top navigation bar includes the c.a.r.u.s. logo, the text 'c.a.r.u.s. HMS GmbH', the 'ViSoR' logo, and the version 'Version V0.1 Build#0020'. The main content area is divided into several sections:

- Pages:** A sidebar menu with options like Project Summary, Assay / Screening Information, Schedule, Deliverables, Additional Comments, and Attachments.
- Actions:** A sidebar menu with options like New, Edit, Save, Refresh, and Cancel.
- General Assay Information:**
 - Reagent Production/Labeling:** A section for defining assay details.
 - Assay Development:**
 - High-content assay:** Includes a dropdown for 'Biochemical assay' (set to 'An assay is available...') and a text field for 'Cellular assay' (set to 'Activators of Prostate Cell Differentiation').
 - Plate format:** Radio buttons for '96-well', '384-well', '1536-well', and 'other'. The '384-well' option is selected.
 - Equipment:** A text field for 'Which equipment was used for performing the assay?' (set to 'PerkinElmer Opera System').
 - Potential Problems:**
 - Technology problems:** A text field (set to 'Plates need to be incubated for 4 days in a humidified, 5% CO2 atmosphere').
 - IP problems:** A text field (set to 'n/a').
 - General Screening Information:**
 - Screening:** A dropdown menu for 'Fragment-based library of 20,000 components'.
 - Profiling:**
 - EC50 determination in same assay:** A text field (set to '10 point dose response assay in triple kits').
 - EC50 determination in different assay:** A text field.
 - Secondary Screens:**
 - Determination of activity in selectivity screen:** A text field (set to 'n/a').
 - Determination of activity in ADMET assay:** A text field (set to 'n/a').

Web technology

The digital workplace ViSoR is founded on a web technology framework with a consistent service-oriented architecture. User-friendly graphical presentation of data structures and a multi-user capability form the core of the application.

Easy to operate

The completely graphical representation with intuitive Windows interfaces requires little training. A researcher can rapidly become familiar with the software package and begin his work with the program quickly and reliably. ViSoR integrates selected third-party systems in a modern and mature overall system, helping you to achieve the highest possible value added for your company.

Grid concept for virtual screening

The integrated virtual screening component is geared towards high-performance cluster- or grid systems. The high computing power of a grid or cluster provides the muscle to screen through molecular databases that comprise of tens of thousand to millions of compounds.

Innovation from c.a.r.u.s.

With ViSoR, the c.a.r.u.s. group developed an IT platform for the early phase of drug development. Import and export of chemical data is handled via specialised interfaces, a wide spectrum of information and data relevant to a project can be collected, stored, and referenced within the system. With an interface to the TrixX program, ViSoR enables reduced virtual-screening run times. ViSoR gives access to high quality results and shortened development times in the search for medically active compounds.

Highlights

- Centralized, consistent database for all users
- Multi-user capability
- Easily integrated interfaces to select third-party systems
- Compatibility with all common file types in pharmaceutical research
- Compound management capability
- Electronic laboratory journal
- Document management (e.g, Word, Excel, etc.)
- User-friendly GUI
- Pure browser-based application
- The latest software architecture SOA improving the seamless and efficient cooperation between applications and services
- State-of-the-art security mechanisms for a Web 2.0 application

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