



## Success Brief

Intel® Xeon® processor  
7400 series

Healthcare  
Data Intensive Computing



“Intel technology was instrumental in the development of the world’s first ‘digital workspace’ analysing the combined results of both wet and virtual high-throughput screening.”

Dr. Matthias Rath,  
managing director,  
c.a.r.u.s. HMS GmbH

## Drug discovery transformed

**c.a.r.u.s. IT AG harnesses the high performance and parallel processing power of the Intel® Xeon® processor 7400 series to run its ViSoR\* platform**

When developing a new small molecule drug, scientists must begin by analysing vast collections of molecules, recording how they react with target proteins. During this process, known as high-throughput screening (HTS), millions of tests are run to identify active compounds able to modulate bio-molecular activities. This screening can be carried out in a laboratory (wet screening) with automated processes on robotic systems, but it is costly and depends heavily upon the quality and quantity of used libraries. An alternative is simulated virtual screening (VHTS) using algorithms, theoretically opening up testing to an unlimited number of molecules; and cutting down on development costs and time to market. Traditionally these two disciplines have stood alone, and scientists have only rarely combined wet and virtual screening results – due to the character of their different approaches. To improve this process, c.a.r.u.s. IT AG has developed a new browser-based IT platform called ViSoR\* (Virtual Screening optimising the Reality), which by its very design integrates both sets of results.

- **Ground-breaking platform:** Develop a web-based platform for scientists involved in drug discovery that would automatically present the findings of both wet and virtual screening in an easy-to-understand, visual format
- **Optimum performance:** Harnessing the high performance and parallel processing capability of the Intel® Xeon® processor 7400 series, c.a.r.u.s. IT AG was able to develop and optimise the performance of ViSoR\* – its new ‘digital workspace’ for high-throughput screening
- **Superior results:** Running ViSoR on Intel® multi-core technology allows researchers to carry out better, more in-depth analysis in a shorter period of time, leaving them free to concentrate on their day-to-day work. Ultimately accelerating and improving the drug discovery process

ViSoR\* brings together a series of applications and databases, including TrixX virtual screening software and a molecular modelling database from the University of Hamburg’s Center for Bioinformatics, which comprises about 10<sup>6</sup> compounds.

For the optimal use and integration of TrixX technology into the ViSoR platform, c.a.r.u.s. IT AG selected Sun Fire X4450 servers, powered by the Intel® Xeon® processor 7400 series with six cores. An alternative was to use a grid-computing system but this would have added additional expense and management complexity, and c.a.r.u.s. IT AG would have had to share the facility with other users. Using a dedicated Sun/ Intel-based system provides sufficient and predictable access to processing power.

TrixX is a multi-threaded application and thus makes optimum use of Intel® multi-core technology, analysing different compounds simultaneously on individual cores. The Intel® Xeon® processor 7400 series also delivers superior performance, taking just ten milliseconds to process one compound on one core. And with a RAM capacity of 10-30 GB, lends itself to running TrixX, which requires enormous amounts of hard disk space.

# Intel® multi-core technology allows for the simultaneous analysis of multiple compounds

It is for these reasons that c.a.r.u.s. IT AG will recommend its customers to run ViSoR on the Intel Xeon processor 7400 series for optimal performance. The x86-based Intel architecture also makes it very easy for organisations to scale the ViSoR platform as workloads increase, and it is compatible with the majority of most common HTS software applications.

The European ScreeningPort is the first customer to sign up to the beta version of ViSoR. As a public private partnership and mainly funded by the German Federal Ministry of Education and Research, ScreeningPort offers the European biomedical research community access to state-of-the-art pharma lab facilities that they would otherwise be unable to access. ScreeningPort was attracted to ViSoR for a number of reasons.

The virtual screening component allows the analysis of an infinite number of compounds and opens up new opportunities – as opposed to wet screening where the number is restricted due to cost, facility and time constraints. Not only does ViSoR automatically combine the results of wet and virtual screening; it also presents data as 2D or 3D graphics which are much easier to interpret than spreadsheets – the old-fashioned way of presenting results especially in academic settings.

ViSoR also facilitates collaboration between ScreeningPort, its academic customers and other partners. Carsten Claussen, CEO at European ScreeningPort, explains: “We should not underestimate ViSoR’s benefits as communication platform: In one of our consortium projects, where our colleagues at the Fraunhofer Institute develop nano particles

## Spotlight: c.a.r.u.s. IT AG

- Established in 1987, c.a.r.u.s. Information Technology AG has offices in three locations in Germany as well as a branch in Romania
- The company focuses on high performance solutions in IT, offering comprehensive software and system solutions for the public healthcare sector and life science industry
- In the life sciences and healthcare sector, c.a.r.u.s. IT AG has a strong focus on working closely with market-leading companies to continuously develop and fine-tune its offering
- The vision of c.a.r.u.s. Healthcare is to close the gap between molecular research and patient therapy, to provide patients with individual treatments optimised for their unique genetic setup or type of illness



for drug deliveries, ScreeningPort executes the lab work. Using ViSoR we are able to discuss results of this lab work in real-time, and can easily change parameters of the test and immediately start the production of new nano particles. Based on this experience, we will extend secure access to ViSoR so all consortium members can collaborate to further refine the biological test system. This was not possible previously.”

Since ScreeningPort runs visualisation software and evaluation tools in parallel with ViSoR, it reaps maximum benefit from the parallel processing power of the Intel Xeon processor 7400 series. ScreeningPort estimates that it will be able to reduce the time taken to visualise the combined results of virtual and wet screening by 25 percent, and will be able to increase the number of compounds it can analyse by a factor of five.

It will be able to carry out more in-depth research projects in a shorter period of time – thus improving and accelerating research into finding new starting points for drug discovery, and attracting more academic customers. The better documented and controlled workflow will reassure pharma companies willing to invest, something academic screening did not always achieve.

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