

## OSIRIS, an entirely in-house developed drug discovery informatics system

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We present OSIRIS, a drug discovery informatics system entirely self-developed at Actelion Pharmaceuticals Ltd. OSIRIS covers all information handling aspects from compound synthesis via biological testing to preclinical development. Its design principles were platform and vendor independence, a consistent look and feel, and complete coverage of the drug discovery process by custom tailored applications. These include electronic laboratory notebook applications for biology and chemistry, tools for high-throughput- and secondary screening evaluation, state-of-the-art chemistry-aware data visualization, physicochemical property prediction, 3D-pharmacophore comparisons, interactive modeling and computing grid based ligand-protein docking. Most applications were written in Java and built on top of a Java library layer that provides reusable functionality and GUI components such as structure canonicalization, combinatorial enumeration, chemical editors, etc.

We use an Oracle database as a scalable persistence engine for data and documents. Its search capabilities were extended by writing an Oracle Cartridge to allow for SQL based chemical substructure and similarity searches. We also employ the Oracle ConText Option to allow document full text searches.

Exemplarily we will demonstrate OSIRIS DataWarrior, a chemistry aware data analysis and visualization tool. It provides simultaneous tabular and graphical views on the same data and allows interactive record filtering on numerical, textual or chemical criteria. It opens various file formats or may directly query the research database. DataWarrior is used for diverse tasks such as combinatorial library planning, microarray data analysis, structure activity correlations on multidimensional project data, or HTS data analysis and lead selection.

Concluding we consider our experience a valid prove that a high degree of in-house software development may be a valid alternative even for smaller drug discovery departments versus the supposedly less risky approach of licensing best-of-bread tools and investing substantially into their integration.

Actelion is a 10 years old biopharmaceutical company with 1700 employees of which about 250 work in drug discovery. We have three drugs on the marked, which exceeded CHF 1.3 billion net revenues in 2007.