

AREAS OF EXPERTISE

Scientific Software Development

Algorithm development

Computer Aided Drug Discovery

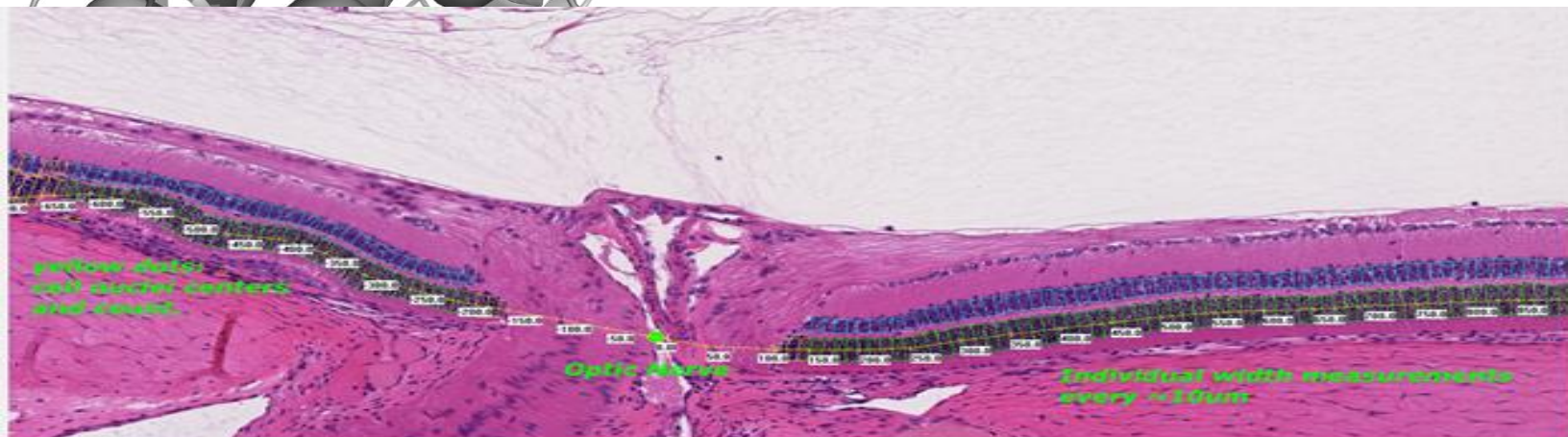
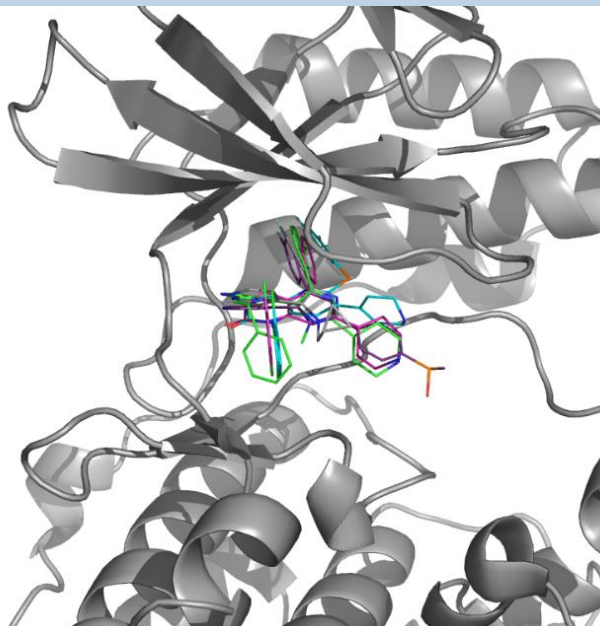
Structure based lead optimization

Virtual Screening: docking pharmacophore based

Screening Library Design

QSAR, QSPR

In silico ADME and Toxicology



Data Analysis

Machine Learning

Predictive Analytics

Data visualization

Cheminformatics

Management Consulting

Infrastructure development

RVision v1.0

Data Table 1 R-Group Table 1

| # | Name | Predicted | Kernel |
|----|--|-----------|-------------|
| 1 | Ridge regression (Gaussian kernel) | Obs logit | Gaussian |
| 2 | Ridge regression (Linear kernel) | Obs logit | Linear |
| 3 | Ridge regression | Obs logit | none |
| 4 | Stepwise forward linear regression | Obs logit | none |
| 5 | Ridge Regression(Fingerprint) | Obs logit | Molecule ht |
| 6 | Stepwise backward linear regression | Obs logit | none |
| 7 | Logistic regression | Obs logit | none |
| 8 | Support vector machine (Linear kernel) | Obs logit | Linear |
| 9 | Support vector machine (Gaussian kernel) | Obs logit | Gaussian |
| 10 | Support vector regression | Obs logit | none |

FACT SHEET

For over 15 years, ALTORIS has been devoted to the advancement and integration of computational tools to accelerate drug discovery efforts. In addition to our products in chemical information management for small molecules and biologics, we provide a wide range of services.

Our services are flexible and range from punctual technical projects to strategic guidance in the drug design arena. Our professional network has a comprehensive view of the full drug discovery cycle that allows our customers to have a part that not only understands the tools but also is familiar with the needs of a drug discovery program.

We have worked over the years with companies in three continents to deliver solutions to their informatics or modeling needs.

SAMPLE CASE STUDIES

- 1) Developed a series of [homology models](#) for a panel of related enzymes to identify pan selective inhibitors. In collaboration with medicinal chemists, docked candidate structures and selected most promising scaffolds for follow-up.
- 2) Aided company in the selection of software to [establish a molecular modeling](#) facility. From delineating requirements to participation in negotiations with vendors, to the training of staff we participated in the entire facility build up process.
- 3) Developed [computer software](#) based on an algorithm designed by us to identify the gross structures of the eye and automate cell counts in each of those structures. Processed the stained tissue slices of rodent eyes, to determine cell viability after blue light exposure and determine the chemoprotective effect of chemicals. This resulted in a considerable time savings when processing the ophthalmic slides.
- 4) Carried out [virtual screening](#) for a kinase target with the ultimate purpose of improving the activity and pharmacokinetic profile of leads identified by HTS.
- 5) [Trained personnel](#) in the techniques for lead hopping when no structural information on the target was available.
- 6) Performed [virtual screening](#) on a GPCR to help in lead optimization.
- 7) Used a combination of [bioinformatics](#) and structural biology techniques to discover a family of peptides that had chemotherapeutic effect against liver cancer.
- 8) Provided [visualization techniques](#) and software integration for a company interested in expanding their capabilities in informatics for biopolymers.