

Lecture: computer assisted procedures

## VirtualToxLab – *in silico* prediction of the toxic (endocrine-disrupting) potential of drugs and chemicals

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The VirtualToxLab is an *in silico* tool for predicting the toxic (endocrine-disrupting) potential of existing and hypothetical compounds (drugs and environmental chemicals) by simulating and quantifying their interactions with the human protein using automated, flexible docking combined with multi-dimensional QSAR. Currently, it includes 11 validated models for the androgen, aryl hydrocarbon, estrogen ( $\alpha/\beta$ ), glucocorticoid, mineralocorticoid, thyroid ( $\alpha/\beta$ ), and peroxisome proliferator-activated receptor  $\gamma$  as well as for the enzymes cytochrome P450 3A4 and 2A13. The models were validated using a total of 824 compounds (630 training +194 test substances). The fully automated technology is accessible through the Internet and allows to mechanistically verify a prediction by interactively inspecting the binding mode of the tested compound(s) with their target proteins in 3D.

The VirtualToxLab is already available for Universities, environmental NPOs and validations centers. By August 1, 2008 public hospitals and regulatory bodies and by October 1, 2008 the Pharmaceutical, Chemical, Biotech, Cosmetics, and Food Industry may benefit from the technology.

Details are given on our website from where the program documentation may be downloaded at <http://www.biograf.ch/downloads/VirtualToxLab.pdf> or the toxic potential of 250+ compounds can be viewed at [http://www.biograf.ch/data/projects/virtualtoxlab\\_results.php](http://www.biograf.ch/data/projects/virtualtoxlab_results.php)

### References

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