

My OpenTox Workshop contribution: The Lost Slides

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During the nice presentations at the recent [OpenTox Workshop](#), I noted that [My OpenTox Workshop contribution: Linking explicit and implicit knowledge](#) was lacking two slides. The slides should have had screenshot of the excellent [Bioclipse](#) applications [Ola Spjuth](#) has written in the area of computational toxicology. But here they are.

Metabolic Fate

The metabolic fate of molecules can be predicted with the [MetaPrint2D](#) feature (see also the [main MetaPrint2D page](#)). The feature currently uses one specific method, but the immediate feedback you get while drawing molecules, can basically use any model. The currently used model is developed in a collaboration of Ola with Sam Adams (whom we all know for his [JNI-InChI](#) library) at Cambridge University and Lars Carlsson at Astra-Zeneca.

The screenshot displays the Bioclipse software interface. On the left, a chemical structure is shown with a silicon atom (Si) bonded to a methyl group, a propyl group, and an oxygen atom. The oxygen atom is part of an ether linkage to a benzene ring. The benzene ring has a nitrogen atom (N) attached to it, which is further connected to a pyridine ring. The pyridine ring has a magnesium atom (Mg) attached to it. The benzene ring is highlighted with green and red circles, indicating metabolic sites. On the right, the 'Welcome' window is open, showing the 'Getting started with MetaPrint2D' tutorial. The tutorial includes an introduction and a list of steps: Step 1: Open the MetaPrint2D Perspective, Step 2: Open a chemical structure, Step 3: Run MetaPrint2D, and Step 4: Examine the results. Below the steps, a detailed explanation of the results is provided: 'MetaPrint2D visualizes the results in a normalized, relative fashion. This means the most likely atom to undergo metabolism is colored RED. Atoms colored ORANGE are moderately likely to undergo metabolism, atoms colored in GREEN are less likely, and atoms with no color have very low probability of metabolism starting in that place. Hover over the atoms to see detailed results on the form: Number of hits in the'.

MetaPrint2D Report

Last MetaPrint2D run

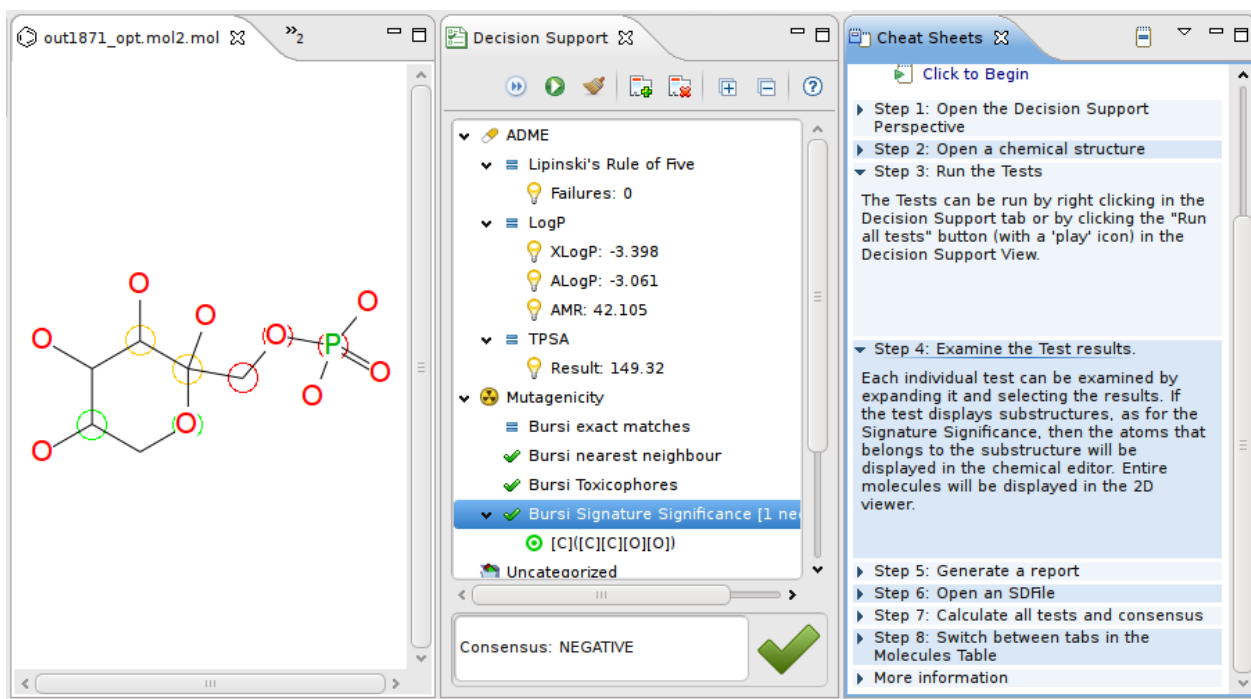
Status	OK
Database	ALL
Operator	DEFAULT
Calculation time	1233 ms

This screenshots shows the visual feedback in the (new) [JChemPaint](#) editor in Bioclipse, and on the right we see one interesting Bioclipse feature in action: the [cheat sheets](#). These cheat sheets are inline help documentation which guides the reader through the functionality. But, unlike mere help, cheat sheets can be very interactive and perform some tasks itself, making it easier for the reader to see what was supposed to happen.

L. Carlsson, O. Spjuth, S.E. Adams, R.C. Glen, S. Boyer, Use of Historic Metabolic Biotransformation Data as a Means of Anticipating Metabolic Sites Using MetaPrint2D and Bioclipse, accepted in BMC Bioinformatics.

Structural Alerts, etc

Structural alerts are one method to signal the scientist that the molecule under study needs some more attention (see for example [doi:10.1016/j.mrrev.2008.05.003](https://doi.org/10.1016/j.mrrev.2008.05.003)). It helps him decide to continue to look at that particular structure, or to move on. Ola also developed a decision support plugin.



One of the cool features is that, in good Bioclipse habits, deliver a pluggable architecture. This practically means, that anyone can add their own decision rules; those can be added as local software, or as services on a central, institute specific server. The results in this screenshot show that a Bursi AMES data-based model estimates that this molecule is mutagenetic.

O. Spjuth, L. Carlsson, M. Eklund, E.A. Helgee, S. Boyer, Integrated decision support for assessing chemical liabilities, In preparation