THE UNIVERSITY OF MINNESOTA PATHWAY PREDICTION SYSTEM

Lynda Ellis[1], Kathrin Fenner[2], Larry Wackett[3]; [1]Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN 55455, [2]Department of Environmental Chemistry, Eawag, 8600 Dübendorf, Switzerland, [3]Department of Biochemistry, Biophysics and Molecular Biology, University of Minnesota, St Paul, MN 55108; lynda@umn.edu

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Introduction. The University of Minnesota Pathway Prediction System (UM-PPS, http://umbbd.ethz.ch/predict/), began in 2002. It predicts plausible pathways of microbial biodegradation of chemical compounds. Predictions are most accurate for compounds similar to compounds with known metabolism; in environments exposed to air, in moist soil or water, at moderate temperatures and pH, with no competing chemicals or toxins; and the major nutrient for the microbe in these environments, rather than present in trace amounts. Predictions are based on rules (253 in Feb 2013).
Features have been added to the UM-PPS to improve use and accuracy of predictions. The UM-PPS is transitioning to new leadership for future development.

Methods. Features of the UM-PPS include expert-ranked rule aerobic likelihood (very likely, likely, neutral, unlikely, very unlikely); relative reasoning (132 in Feb 2013), which assigns certain rules priority over others (*e.g.* ring cleavage > ring oxygenation); super rules (22 in Feb 2013), one rule based on contiguous rules that make up a small pathway of their own (*e.g.* bt0351, super rule for extradiol ring cleavage); variable aerobic likelihood (27 in Feb 2013), decreasing aerobic likelihood on substrates with certain chemical structures (*e.g.* substrates with halogens).

Results. The most recent features added include multi-step predictions, improved pathway visualization, a zoom feature, pathway output in both .html and .pdf format, and the ability to delete pathway branches.

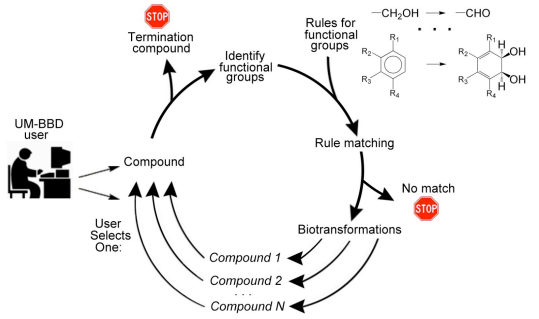

Fig.1 The UM-PPS prediction cycle.

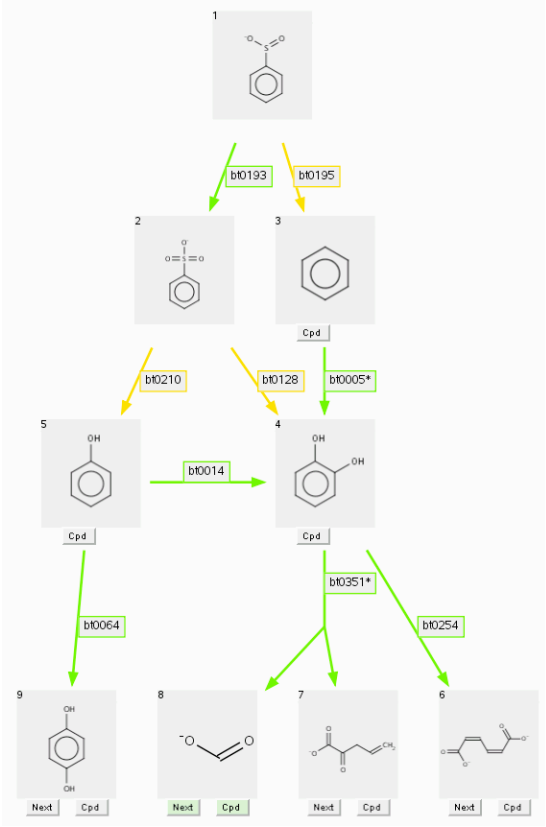

Fig.2 UM-PPS prediction

Conclusions. Future developments include tailoring predictions to different environments.

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References.

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