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PRIORITIZATION OF PREDICTED BIODEGRADATION PATHWAYS USING ENERGY EFFICIENCY ANALYSIS

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ABSTRACT: One important aspect in chemical risk assessment is to assess the extent of exposure to environmental transformation products of the parent compound. For most chemicals, however, their transformation pathways and stable transformation products are barely known. The University of Minnesota Pathway Prediction System (UM-PPS) is a collection of about 250 structure-based transformation rules to predict possible biodegradation pathways of xenobiotics. Due to the broad applicability of some of the rules, UM-PPS produces a large number of possible transformation products and pathways (combinatorial explosion). The work presented investigates whether energy efficiency of predicted pathways can be used as a criterion to determine the likelihood of different predicted microbial degradation pathways. To this end, the production of reducing power during oxidation steps leading to final mineralization of xenobiotics is expressed in terms of ATP yields, with ATP used as general energy currency. ATP yields of known pathways are compared to those of all possible pathways predicted by UM-PPS and the hypothesis that the former generally exhibit ATP yields at the upper end of the entire prediction interval is tested for five case-study compounds (glyphosate, atrazine, diuron, MTBE, and nitrilotriacetic acid (NTA)).Complete transformation schemes were generated for these compounds, yielding 14, 27, 22, 148 and 280 transformation products and 132, 2,223, 8,444, 1,977,448, and 374,052,438 possible biodegradation pathways for glyphosate, diuron, NTA, MTBE and atrazine respectively. ATP counts were attributed to the UM-PPS transformation rules triggered in the transformation schemes, based on the knowledge of classes of enzymes associated with the single rules, and summarized over each possible pathway. The results indicate that ATP yields of known pathways generally lie in the top 20th percentile range of the entire prediction interval. Reducing the prediction space of possible transformation pathways to those that yield ATP counts in the upper 20th percentile region reduced the number of predicted transformation products by about one fifth. The approach developed can thus be useful as a criterion, amongst others, to focus monitoring and risk assessment of transformation products on those that have a high likelihood of being formed through microbial biodegradation.

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