

# Use and value of metabolism databases

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„...products currently exist, **MetabolExpert 18 (CompuDrug, Budapest, Hungary)** and **META**...also be readily excreted. **MetabolExpert** excludes phase II metabolites...pharmacologically or toxicologically. **MetabolExpert** incorporates the provision...”

## Abstract

A key objective during drug discovery is to ensure selection of lead compounds for development that have the optimum pharmacodynamic profile without undesirable toxicity. Metabolism plays a key role in determining the biological activity of compounds *in vivo*, and is therefore an important factor to consider during the discovery phase. The ability to predict the biotransformation pathways for specific chemical structures provides the opportunity to implement structural modifications that might advantageously modify these processes. Potentially valuable tools include knowledge databases that contain searchable information on the known metabolites of existing compounds and databases that are designed to predict the metabolites.

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