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EDITORIAL

A user-friendly guide on how to obtain and accurately interpret information from metabolic databases

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In the past years, the use of bioinformatical and modelling techniques in research has dramatically increased. Examples of applications include the identification of overrepresented transcription factors and biological functions of differentially expressed genes (Glahn et al. 2008; Godoy et al. 2009; Cadenas et al. 2010; Zellmer et al. 2010; Meyer et al. 2011), the establishment of pharmacokinetic and quantitative structure–activity models (Gundert-Remy et al. 2009; Bolt and Hengstler 2010; Hengstler et al. 2011; Mielke et al. 2011) or spatial–temporal models (Hoehme et al. 2007; 2010).

Even within the pages of our journal, the number of published papers on modelling has also increased in recent years (Lilienblum et al. 2008; Keller et al. 2009; Lehmann et al. 2010; Rupp et al. 2010; Golka et al. 2011). Therefore, experimentalists in the field of Toxicology can only gain if databases and bioinformatics are properly integrated into their experimental work. Unfortunately, this is currently not the case as many scientists may be discouraged by the complexity and missing user-friendliness of such databases. Therefore, it is highly appreciated that Karp and Caspy (2011; this issue) from the Bioinformatics Research Group in California accepted our invitation to contribute a review on metabolic databases. The review not only gives an overview of the numerous databases presently available, but also provides a user-friendly introduction for those not yet familiar with this type of software tools. Examples of 'quick search' queries which can be accomplished, even by beginners, within less than 5 min include as follows:

- Enter a metabolite of interest. The software will then show all known pathways on how this metabolite is further processed. For example, entering 'L-lysine' generates three pathways, two on the degradation of L-lysine and one tRNA charging pathway.
- Enter a gene or enzyme of interest. A 'regulation software' will then show all metabolites or protein factors that are involved in its regulation. For example, when the trpA gene is entered, tryptophan is highlighted because it also functions as a regulator at the transcriptional level. The software also returns the compound pyridoxal phosphate that activates the trpA, in addition to a small RNA molecule controlling translation of the trpA mRNA.
- Enter a pathway. The software will return all known enzymes involved. For example, upon entering 'glycolysis', the software shows 40 enzymes and their respective activities, which is certainly more than can be found in current textbooks or reviews.

Besides those easy to handle aspects, more complex functions can be processed, for example, the overlay of transcriptional datasets with metabolic activities. The review is a must-read for anyone interested in metabolic pathways and networks.

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