

A Computer Experiment Model to Investigate the Effects of Drug Dosage in Animals, for Use in Pharmacological Education and Research

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Summary — The ACD-IDEA database, which was originally developed by the authors in 2004, is an ongoing compilation of existing data on the *in vivo* doses of compounds at which various responses in certain animal species have been observed. It can provide an infrastructure for various research/educational efforts, and creates a synergy for new applications. In this paper, some of these applications are described. Specific interfaces within the database are designed for users who are not computer specialists. Users can search the database to find the answer to a query, or they can design a simple virtual animal experiment. In the second case, the interface is used to undertake a dialogue with the system, in order to test the user's knowledge regarding an experiment under consideration, and to allow the user to glean additional information on better experimental planning. The use of this virtual experimental tool should lead to savings in time, animals, materials, and monetary costs, while the effective learning outcomes of pharmacological experiments are maintained or enhanced.

Key words: computer experiment, drug-dosage data, educational tools, laboratory animal experiment.

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Introduction

The ACD-IDEA database, originally developed by the authors in 2004 (1, 2), is an ongoing compilation of data on the *in vivo* doses of compounds at which various responses in certain animal species have been observed. This kind of collation and review of existing data is very important for all sciences. In the fields of fundamental and applied experimental science, the amount of data is immense, having been obtained over a long period of time. There are also enormous process and material costs associated with the acquisition of such a volume of data. Hence, improved processes are necessary to extract the precise data and the knowledge we need from them. Computer tools can assist in solving these types of problems. When considering a large amount of data, database applications can be implemented that are capable of storing, maintaining, distributing, and sharing the data (3, 4). One of the most important advantages of using appropriately designed computer database applications for such a large amount of data, is that one can obtain new data from a limited number of additional experiments, or sometimes even with no additional experiments at all. Some of these computer databases permit the application of expert systems (4), and give the user the capability of conducting virtual experiments based on the data within them. The availability of

databases for use in new drug research and development is also important, and this importance will increase in the future, as the costs and complexities involved in drug discovery and development continue to increase (5). Indeed, in order to enhance and augment classical laboratory research, it is foreseen that many computer-aided applications will need to be developed for use in the field of pharmacological research (6).

Pharmacological research and education covers a wide range of considerations. One of them is the *in vivo* determination of drug-dosages for application to different experimental animals. Many types of drugs are applied to a range of experimental animals via different administration routes, at various dosages, producing basic exposure data for the individual parameters that are tested. In many instances, these experiments produce very different and contradictory results. It is imperative that such data should be registered, published and shared among those involved in the field, to avoid unnecessary duplication of efforts and repetition of experiments. Often, similar experiments producing the same data are repeated continuously throughout the world, at least for educational or research purposes.

The number of registered and published pharmacological experiments is extensive, and covers a period of almost 100 years (7, 8). The ACD-IDEA database was developed for the collation of many of