



ADME DB is a database containing the latest and most comprehensive data on interactions of substances with Drug Metabolizing Enzymes and Drug Transporters. It is designed for use in drug research and development, including drug-drug interactions and ADME (Absorption, Distribution, Metabolism and Excretion) studies. The information is organized by category (therapeutic area), drug name, enzyme, reaction, and type. ADME DB is supported by chemical/metabolite structures as well as kinetic values found in the literature. The database is available online and completely searchable by keywords or chemical structures. Advanced searches are also available to support investigational studies on drug-drug interactions.

Human Drug Metabolizing Enzymes Database

- Provides information on specific interactions for a given substance with Human Phase I Enzymes such as P450 (CYP), FMO, AKR, MAO and AO; Human Phase II Enzymes such as Esterases, UGT, GST, and SULT.
- Contains over 33 000 entries.
- Contains more than 15 700 substances, a number of natural products and preparations,



as well as other factors influencing Drug Metabolizing Enzymes activity.

- Contains data collected from more than 6 200 citations.



Kinetic Metabolism Database

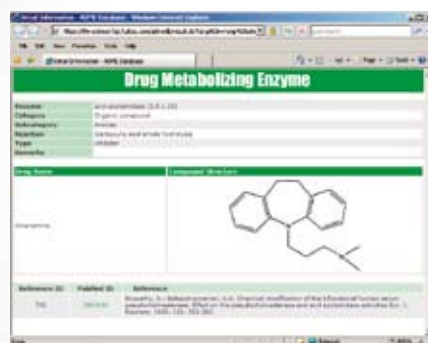
- Database contains over 26 000 entries extracted from Human Cytochrome P450 metabolism database references providing numerical data on major kinetic parameters relevant for use in drug developing/application studies.

Human Transporters Database

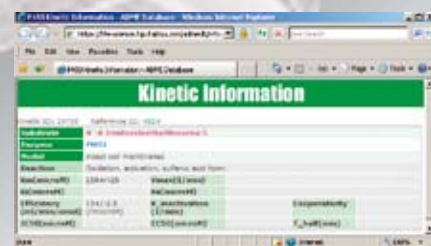
- Provides information on more than 250 Transporters (including ABCs, OATPs, OCTs, OATs, SLCs) involved in drugs transport, physiological compounds, nutrients, and other chemicals and metabolites.
- Contains over 12 000 entries.
- Contains data collected from ~ 3 280 citations.

Examples of applications of the system

- Evaluating and predicting clinical side effects and interactions of known and new drugs/chemicals/physiological compounds.



- Computer assisted development of new drugs and pro-drugs.
- Selecting CYP-selective substrates/inhibitors for in vivo/in vitro studies.
- Studying properties of natural and artificial CYP mutants using selective metabolic reactions.



Hardware and software requirements Server

- Suggested hardware configuration: Intel Pentium 4 2.0 GHz or higher; 512 MB RAM or more; 500MB HDD space or more.
- Operating systems: UNIX, Windows 2000/XP, and Red Hat Linux 9 or higher.
- Apache Software Foundation Tomcat 4.1.12 or higher.
- PostgreSQL 7.3.2 or higher.
- Java JDK 1.4.2 or higher.

Client

- Microsoft Internet Explorer 5.5sp2 or higher or Netscape Communicator 4.75 or higher.