Resource Summary Report

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Drug ADME Associated Protein Database

RRID:SCR_013501 Type: Tool

Proper Citation

Drug ADME Associated Protein Database (RRID:SCR_013501)

Resource Information

URL: http://xin.cz3.nus.edu.sg/group/admeap/admeap.asp

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Description: A database for facilitating the search for drug Absorption, Distribution, Metabolism, Excretion (ADME) associated proteins. It contains information about known drug ADME associated proteins, functions, similarities, substrates / ligands, tissue distributions, and other properties of the targets. Associated references are also included. Drug absorption, distribution, metabolism and excretion (ADME) often involve interaction of a drug with specific proteins. Knowledge about these ADME-associated proteins is important in facilitating the study of the molecular mechanism of disposition and individual response as well as therapeutic action of drugs. It is also useful in the development and testing of pharmacokinetics prediction tools. Several databases describing specific classes of ADMEassociated proteins have appeared. A new database, ADME-associated proteins (ADME-AP), is introduced to provide comprehensive information about all classes of ADMEassociated proteins described in the literature including physiological function of each protein, pharmacokinetic effect, ADME classification, direction and driving force of disposition, location and tissue distribution, substrates, synonyms, gene name and protein availability in other species. Cross-links to other databases are also provided to facilitate the access of information about the sequence, 3D structure, function, polymorphisms, genetic disorders, nomenclature, ligand binding properties and related literatures of each protein. ADME-AP currently contains entries for 321 proteins and 964 substrates. ADME Class Based on their respective role of pharmacokinetics, ADME-associated proteins can be classified into four categories: A: This Category includes proteins involved in the absorption or re-absorption of drugs into systemic system. D: This category includes proteins responsible for facilitating the distribution of drugs from the systemic system to the target sites or away from the target sites back to the systemic system. Certain plasma proteins and intracellular binding proteins may alter free drug concentration by acting as drug storage depot. These proteins thus play a regulatory role in drug distribution and they are thus

included in Category D. Based on their role in drug distribution, proteins in this category can be further divided into three groups D1, D2, and D3. The first group D1 includes transporters capable of transporting chemicals across membranes of various tissue barriers from the systemic system into the target sites. Blood-brain barrier and placenta barrier are examples of tissue barrier. Proteins in the second group D2 are responsible for transporting drugs back into the systemic system. Proteins in the third group D3 mainly function as drug storage depot. These include ligand binding proteins in plasma and intracellular proteins. M: Proteins in category M are drug-metabolizing enzymes. These enzymes can be further divided into two separate groups M1 and M2, according to whether the corresponding enzymatic reaction is phase I or phase II. E: This category E includes proteins that enable the excretion or presystemic elimination of drugs. Some proteins belong to more than one category: e.g. Pglycoprotein both limits intestinal absorption and excludes drugs from the brain back to the blood. It thus belongs to both Category E and D. For those proteins capable of transporting natural substrates without literature report of interaction with a drug, a postfix potential is attached to their respective classification to indicate that their specific role in ADME is yet to be confirmed. Use of ADME-AP for commercial purposes is not allowed.

Synonyms: ADMEAP

Resource Type: data repository, storage service resource, data or information resource, service resource, database

Keywords: drug, drug-metabolizing enzymes, elimination, excretion, functions, absorption, distribution, intracellular proteins, ligand binding proteins, ligands, metabolism, pharmacokinetics, protein, similarities, substrates, targets, tissue distributions, transporters

Funding:

Resource Name: Drug ADME Associated Protein Database

Resource ID: SCR_013501

Alternate IDs: nif-0000-21131

Record Creation Time: 20220129T080316+0000

Record Last Update: 20250513T061447+0000

Ratings and Alerts

No rating or validation information has been found for Drug ADME Associated Protein Database.

No alerts have been found for Drug ADME Associated Protein Database.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 3 mentions in open access literature.

Listed below are recent publications. The full list is available at <u>NIF</u>.

Chuntakaruk H, et al. (2024) FMO-guided design of darunavir analogs as HIV-1 protease inhibitors. Scientific reports, 14(1), 3639.

Choi GW, et al. (2019) Interpretation of Non-Clinical Data for Prediction of Human Pharmacokinetic Parameters: In Vitro-In Vivo Extrapolation and Allometric Scaling. Pharmaceutics, 11(4).

Pearce CL, et al. (2017) Pharmacogenetic Associations with ADME Variants and Virologic Response to an Initial HAART Regimen in HIV-Infected Women. International journal of HIV/AIDS and research, 4(3), 154.