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Human *In vitro* Drug Transporter Dataset

Transforming scientific data into clinical knowledge

The Drug Transporter Dataset contains results from *in vitro* transporter studies, where a drug is tested as an inhibitor (precipitant) or a substrate (object) for a given human drug transporter (including variants).

- **Transporter parameters** (IC_{50}, K_i, % inhibition, P_{app}, efflux ratio, uptake ratio, K_m, and V_{max}) and *in vitro*-to-*in vivo* prediction ratios per FDA DDI guidance, along with detailed experimental conditions, are extracted from published articles (citations) and NDA/BLA reviews.

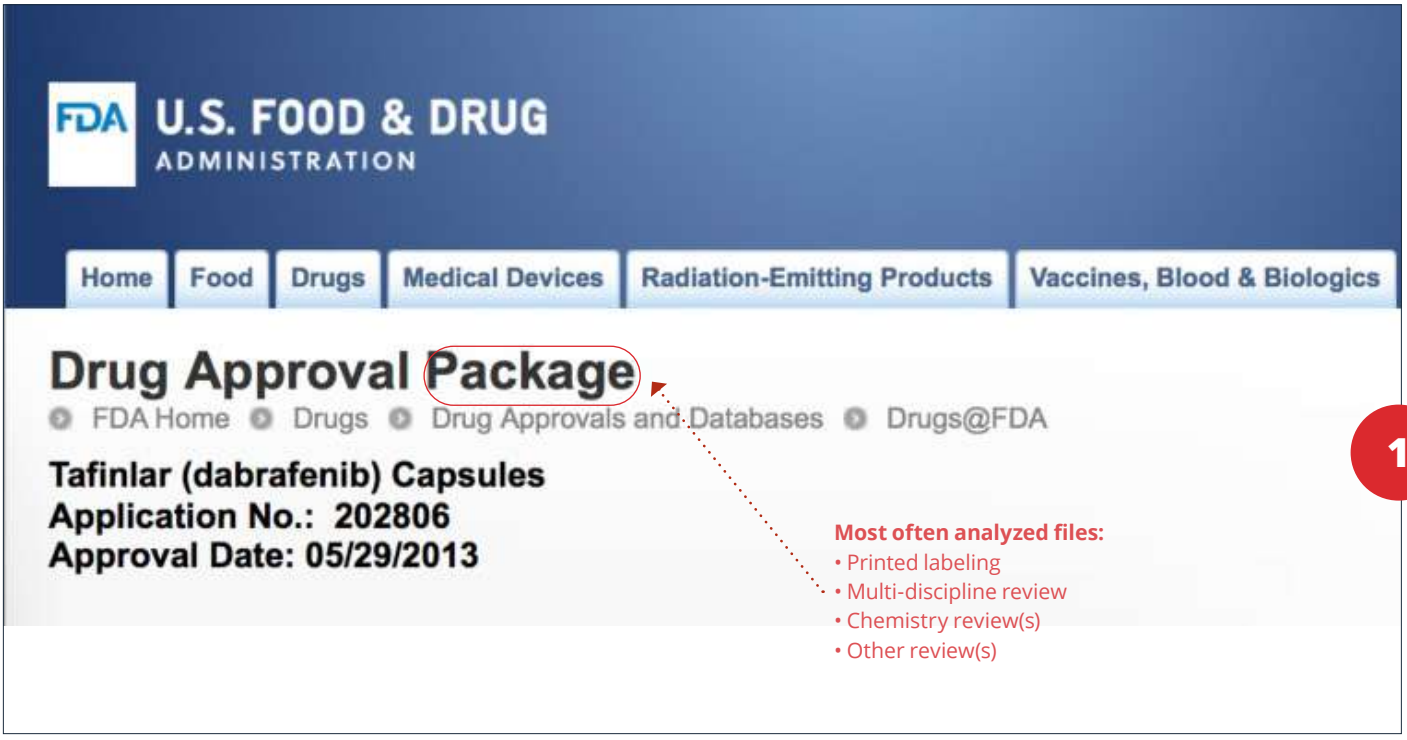
- **Study results** are organized according to the overall effect and mechanism of the interaction:
  → Transporter inhibition entry: drug as inhibitor or non-inhibitor
  → Transporter substrate entry: drug transported or not transported

- **Multiple queries** allow users to retrieve an *in vitro* dataset by drug name, transporter name, or mechanism of the interaction (drug as inhibitor or as substrate).

- **Results** can be viewed, customized, and downloaded in multiple formats, allowing users to compile and organize the large body of information available.

FROM A **CITATION** OR **NDA/BLA REVIEW**

The latest, most relevant, peer-reviewed publications and regulatory documents are identified and fully analyzed. Study protocol and results are manually curated to update the knowledgebase on a daily basis.



TO A FULLY **CURATED DATASET**

Prior to integration, all data are carefully and critically evaluated. The richness of each citation, including relevant insights, is exploited, generating a highly detailed dataset.

Tree View of Citation Data

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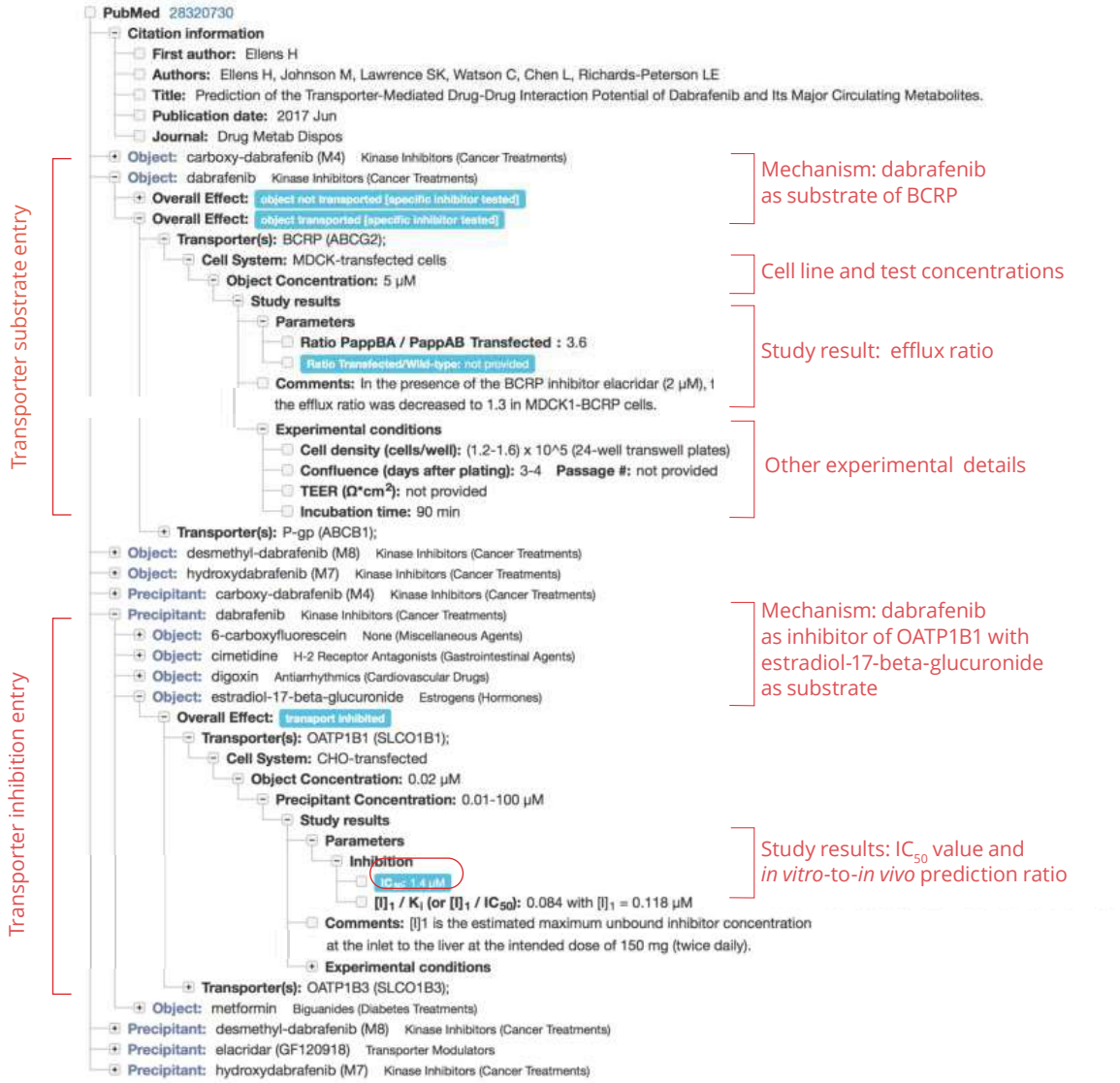

Dabrafenib inhibits OATP1B1 with an IC_{50} value of 1.4 µM.
What other OATP1B1 inhibitors have IC_{50} values ≤ 10 µM?

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POWERFUL TOOL FOR **DATA INTEGRATION**: FROM ONE CITATION TO METADATA ANALYSIS

The data are formatted for immediate use and can be filtered and re-arranged to allow meta-analysis of multiple results.

Query all OATP1B1 inhibitors with IC_{50} ≤ 10 µM

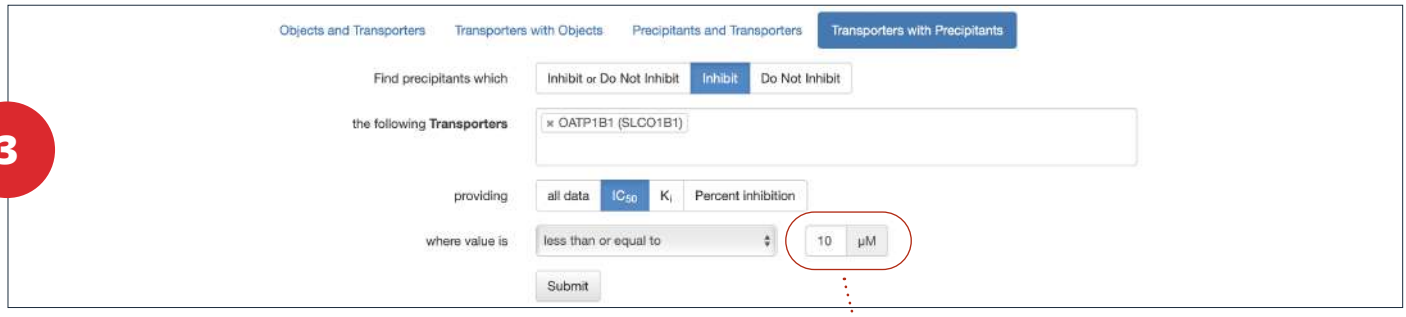

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Table View of Query Results

Filter

Multiple formats for viewing and downloading

Showing 1 to 100 of 263 entries (filtered from 771 total entries)

Advanced Table Search | Select columns | Copy | Excel | CSV | Print

Precipitant	Precipitant Therapeutic Class	Object	System	Object Concentration	Precipitant Concentration	IC_{50} (µM)	Accession # or NDA/BLA #	Published
		estrad ×				-		
bilirubin ditaurate	Miscellaneous Agents → None	estradiol-17-beta-glucuronide	HEK293-transfected cells	2 µM		0.005	**PubMed** 19560444	2009 Nov 10
glecaprevir	Treatments of AIDS → Protease Inhibitors	estradiol-17-beta-glucuronide	Membrane vesicles	2.0 µM		0.017	**PubMed** 31167814	2019 Aug
cyclosporine	Immune System Agents → Immunosuppressants	estradiol-17-beta-glucuronide	HEK293-transfected cells		0.003 to 6 µM (30-45 min of pre-incubation)	0.019	**PubMed** 23179780	2013 Mar
rifamycin	Anti-Infective Agents → Antibiotics	estradiol-17-beta-glucuronide	HEK293-transfected cells	0.02 µM	0.001-30 µM	0.02	**PubMed** 26700956	2016 Mar
rifamycin	Anti-Infective Agents → Antibiotics	estradiol-17-beta-glucuronide	HEK293-transfected cells	2 µM	0-50 µM (estimated from Fig. 2A)	0.05	**PubMed** 23886114	2014 Mar
cyclosporine	Immune System Agents → Immunosuppressants	estradiol-17-beta-glucuronide	HEK293-transfected cells	0.02 µM	0.01-3 µM	0.05	**PubMed** 17901929	2008 May

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Obtain a complete list of *in vitro* inhibitors of OATP1B1

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IN VITRO TRANSPORTER DATASET IN NUMBERS

(as of October 16, 2023)

3,248 citations / **350** NDAs/BLAs

16,953 substrate entries / **41,055** inhibition entries

38,259 positive entries / **19,749** negative entries

Dedicated *in vitro* transporter queries with **26** possible searches

108 drug transporters & **38** variants

2,543 compounds as substrates / **4,837** compounds as inhibitors

569 food products & **1,002** herbal medications

APPLICATIONS OF THE IN VITRO METABOLISM DATASET

PROVIDES CONTEXT for RESULTS OBTAINED with candidate compouds

ALLOWS ASSESSMENT of MEASUREMENT VARIABILITY
(inter-lab, substrate- and system-dependency, etc.)

SUPPORTS STATIC PREDICTIONS and PBPK MODELING
with input parameters

HELPS OPTIMIZE *IN VITRO* STUDY DESIGN
(cell system, incubation conditions, test concentrations, choice of substrate/inhibitor, etc.)

ASSISTS with DOSE SELECTION for clinical trials

PROVIDES *IN VITRO* EVIDENCE to EXPLAIN CLINICAL RESULTS and improve understanding of drug interaction mechanisms

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To learn more, visit www.druginteractionsolutions.org

or email DIDBase@Certara.com

About Certara

Certara accelerates medicines using proprietary biosimulation software, technology and services to transform traditional drug discovery and development. Its clients include more than 2,000 biopharmaceutical companies, academic institutions, and regulatory agencies across 62 countries.

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