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DRUG METABOLISM & DISPOSITION

Special Section on Natural Products: Experimental Approaches to Elucidate Disposition Mechanisms and Predict Pharmacokinetic Drug Interactions

A New Data Repository for Pharmacokinetic Natural Product-Drug Interactions: From Chemical Characterization to Clinical Studies[S]

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ABSTRACT

There are many gaps in scientific knowledge about the clinical significance of pharmacokinetic natural product–drug interactions (NPDIs) in which the natural product (NP) is the precipitant and a conventional drug is the object. The National Center for Complimentary and Integrative Health created the Center of Excellence for NPDI Research (NaPDI Center) (www.napdi.org) to provide leadership and guidance on the study of pharmacokinetic NPDIs. A key contribution of the Center is the first user-friendly online repository that stores and links pharmacokinetic NPDI data across chemical characterization, metabolomics analyses, and pharmacokinetic in vitro and clinical experiments (repo.napdi.org). The design is expected to help researchers more easily arrive at a complete understanding of pharmacokinetic NPDI research on a particular NP. The repository will also facilitate multidisciplinary collaborations, as the repository links all of the experimental data for a given NP across the study types. The current work describes the design of the repository, standard operating procedures used to enter data, and pharmacokinetic NPDI data that have been entered to date. To illustrate the usefulness of the NaPDI Center repository, more details on two high-priority NPs, cannabis and kratom, are provided as case studies.

SIGNIFICANCE STATEMENT

The data and knowledge resulting from natural product–drug interaction (NPDI) studies is distributed across a variety of information sources, rendering difficulties to find, access, and reuse. The Center of Excellence for NPDI Research addressed these difficulties by developing the first user-friendly online repository that stores data from in vitro and clinical pharmacokinetic NPDI experiments and links them with study data from chemical characterization and metabolomics analyses of natural products that are also stored in the repository.

Introduction

Natural products (NPs) include herbal and other botanical products (Paine and Roe, 2018). Pharmacokinetic interactions involving NPs and conventional [e.g., approved by the US Food and Drug Administration (FDA)] drugs could result in reduced treatment efficacy or adverse effects (Paine et al., 2018). Although up to 88% of older adults use herbal medicinal products concurrently with conventional drugs (Batanero-Hernán et al., 2017), there are many gaps in scientific knowledge about the clinical significance of pharmacokinetic NP–drug interactions (NPDIs) in which the NP is the precipitant and a conventional drug is the object. Although 6 of the 40 top-selling herbal medicinal products in 2017 were implicated in clinically significant pharmacokinetic NPDIs, there was minimal or no supporting clinical evidence for potential NPDIs involving nine products (Spanakis et al., 2019). Similarly, data were insufficient to conclude the clinical relevance of 11 of the 15 potential pharmacokinetic NPDIs involving antiretroviral drugs (Fasinu et al., 2015).

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ABBREVIATIONS: CBD, cannabidiol; FAIR, findable, accessible, interoperable, and reusable; FDA, US Food and Drug Administration; NaPDI Center, Center of Excellence for Natural Product–Drug Interaction Research; NP, natural product; NPDI, NP-drug interaction; P450, cytochrome P450; SOP, standard operating procedure; THC, tetrahydrocannabinol; UGT, UDP-glucuronosyltransferase.

There are several unique challenges associated with pharmacokinetic NPDI research, including the large variability of phytoconstituents among marketed products, difficulty extrapolating results from animal and/or in vitro models to humans, variability in study design, and inadequate methods (Paine et al., 2018). Based on these knowledge gaps and challenges, the National Center for Complimentary and Integrative Health created the Center of Excellence for NPDI Research (NaPDI Center; www.napdi.org) to provide leadership and guidance on the study of pharmacokinetic NPDIs (Paine et al., 2018).

One objective of the NaPDI Center is to develop and apply a set of Recommended Approaches to determine the clinical relevance of pharmacokinetic NPDIs (Johnson et al., 2018; Paine et al., 2018; Kellogg et al., 2019). A key deliverable of the Center is the development of an online repository for data generated by the NaPDI Center (repo.napdi.org). The repository combines data currently distributed across a variety of information sources into a single user-friendly format complemented by an information portal. This portal, also developed by the NaPDI Center, disseminates the Recommended Approaches (Johnson et al., 2018; Paine et al., 2018; Kellogg et al., 2019) on the optimal conduct of pharmacokinetic NPDI studies (napdicenter.org). Combined, these new resources will help advance pharmacokinetic NPDI research by providing Recommended Approaches and novel pharmacokinetic NPDI data.

Pharmacokinetic NPDI data include chemical characterization of NPs, metabolomics analyses, and in vitro and clinical pharmacokinetic experimental results. This new repository stores data from all of these types of investigations. It provides a user-friendly interface that enables users with limited informatics skills to effectively explore relevant data (Li, 2015). As of March 2020, coverage of the repository is limited to four carefully selected high-priority NPs based on a systematic method for the purpose of demonstrating the Recommended Approaches (Johnson et al., 2018): cannabis (*Cannabis sativa*), goldenseal (*Hydrastis canadensis*), green tea (*Camellia sinensis*), and kratom (*Mitragyna speciosa*). A prior Recommended Approach (Johnson et al., 2018) reported the inclusion of licorice (*Glycyrrhiza* spp.). The Center later replaced licorice with kratom to 1) keep pace with public health needs in the face of an ever-changing NP market (Gaston et al., 2020) and 2) omit redundancy with the research efforts of a longstanding botanical center (https://pcrps.pharmacy.uic.edu/our-centers/uic-nih-center-for-botanical-dietary-supplements-research/).

The current work describes the design of the repository, standard operating procedures (SOPs) used to enter data, and pharmacokinetic NPDI data that have been entered to date. To illustrate the usefulness of the NaPDI Center repository, more details on two high-priority NPs, cannabis and kratom, are provided as case studies.

Materials and Methods

Construction and Content

Studies Conducted by NaPDI Center Investigators. To date, the repository has focused on original pharmacokinetic NPDI research conducted by NaPDI Center investigators, who are organized into three cores with complementary expertise (Fig. 1).

The Analytical Core is composed of NP chemists, analytical chemists, and clinical pharmacologists and serves multiple functions. This core chemically characterizes multiple commercially available products of a given NP, determines the contents of constituents in these products, and provides guidance on the proper selection of one or more commercially available products to be tested by the Pharmacology Core. The core also analyzes plasma and urine samples obtained from pharmacokinetic clinical studies for NP constituents and object drugs.

The Pharmacology Core is composed of clinical pharmacologists and medicinal chemists. This core designs and conducts rigorous experiments to evaluate the potential for NPs to precipitate pharmacokinetic interactions with certain object drugs. The core also characterizes the pharmacokinetics of select NP constituents in human subjects. The data obtained are used to develop physiologically based pharmacokinetic models that can be applied to other object drugs and patient populations of interest. Figure 2 shows the variety of different experiment types that the repository supports to store data from the NaPDI Center's interaction projects.

The Informatics Core (Fig. 1) is composed of biomedical informaticists, computer scientists, and communication experts. This core compiles all data generated from NaPDI Center research activities into the data repository, which is accessible via the information portal. Prior to public release, NaPDI Center data are only accessible to researchers approved to access the site. Contributing researchers indicate when to make the data public. The data are made available according to a Recommended Approach for making pharmacokinetic NPDI research data findable, accessible, interoperable, and reusable (FAIR; https://www.w3id.org/hclscg/npdi).

Data Types. A variety of data types are produced from pharmacokinetic NPDI studies (Supplemental Table 1). Initially, the specification and subsequent characterization of the NP source materials generated a diverse set of data, including chromatograms from conventional high-pressure liquid chromatography with UV detection and ultrahigh-pressure liquid chromatography–mass spectrometry methods, spectral data from nuclear magnetic resonance and circular dichroism, and bioactivity fractionation data. These data include instrument tracings that are often not retrievable in digitized form. Hence, the scanned image files are archived in the repository. Quantitative data on NP source materials, such as content of individual phytoconstituents and specific impurities or contaminants, are organized in tabular format.

The types of data generated from in vitro NPDI studies vary across the range of human-derived in vitro test systems, including enzymatic reactions involving recombinant enzymes, human tissue fractions (e.g., human liver microsomes), or cultured cells (e.g., hepatocytes), and drug transport experiments measuring uptake into membrane vesicles or efflux from transfected cells. Currently, the data repository tracks 82 measurements for quantitative data resulting from NPDI experiments. The full list is provided in Supplemental Table 1. Included in the list are, for example, percent inhibition, IC_{50}, K_m, and V_{max}.

In addition, data generated from inhibition experiments involving drug metabolizing enzymes or transporters differ from those generated from induction experiments. Thus, the repository provides separate sets of data fields for each of these in vitro systems and mechanisms (Supplemental Table 1).

Pharmacokinetic data generated from clinical NPDI studies include human subject demographics, concentration-time data, and key pharmacokinetic endpoints (e.g., oral clearance, renal clearance, apparent volume of distribution, half-life, area under the plasma-concentration vs. time curve, maximum plasma concentration, and time to reach maximum concentration). Statistical analyses of primary and secondary pharmacokinetic endpoints generated additional data sets.

Data Findability, Accessibility, Interoperability, and Reusability. There is a growing recognition by both researchers and funding agencies that pharmacokinetic NPDI study data sets should be more FAIR (National Center for Complementary and Integrative Health, 2019). The NaPDI Center repository is designed to ensure that data satisfy these four foundational principles of good data management and stewardship. Table 1 summarizes the specific features of the repository that support FAIR pharmacokinetic NPDI data. Each feature is described in greater detail in a public and participative report that the NaPDI Center is developing in collaboration with the World Wide Web Consortium Semantic Web in Health Care and Life Sciences Community Group (https://www.w3id.org/hclscg/npdi).

Standard Operating Procedures for Data Entry. A major feature of the repository is that data are entered using validated SOPs. There are currently 11 SOPs, one for each experiment type listed in Figure 2. Data collection forms have been developed for both internal and external NPDI researchers, such as contract research organizations. These forms are based closely on the SOP documents. Both the SOPs and data entry forms are publicly available on GitHub (https://github.com/dbmi-pitt/NaPDI-SOPs), and the SOP document for enzyme inhibition experiment type is provided as an example in Supplemental Data (Boyce et al., 2020).

Quality Control and Validation Processes. Given the variety of data types, close attention must be paid to enable accurate tracking and meticulous organization of the generated data. The structure, data organization, and concepts effectively used by the University of Washington's Drug Interaction Database (Hachad et al., 2010), now Drug Interaction Solutions (www.druginteractionsolutions.org), have been

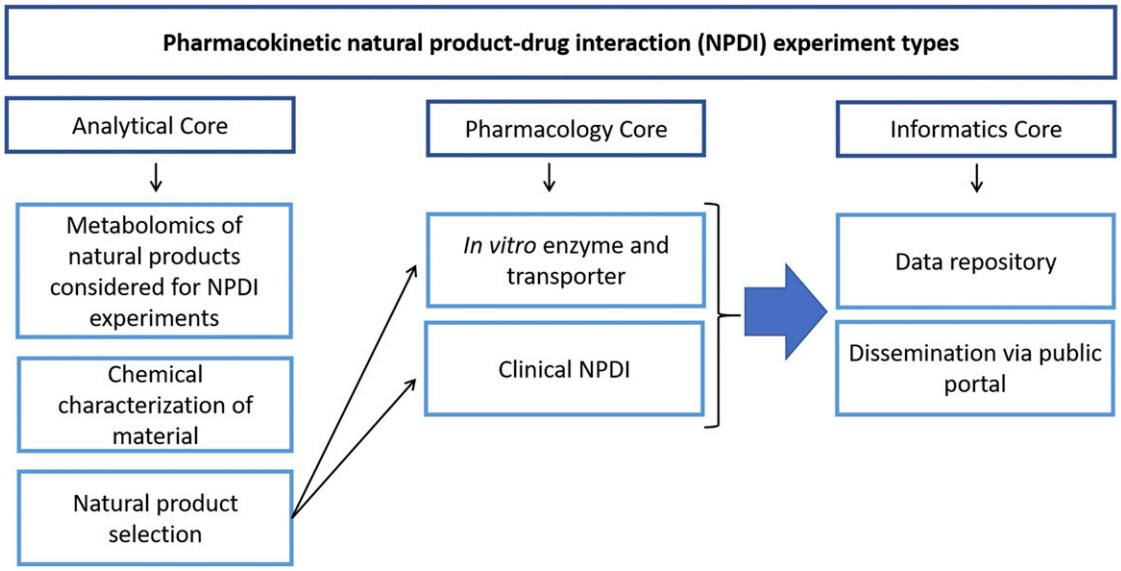

Fig. 1. Types of pharmacokinetic NPDI experiments conducted by the NaPDI Center.

applied to the NaPDI Center repository. These features have been validated over time with feedback from a large user base. To ensure the quality and consistency of the entry process, data are entered by experienced curators who are well versed in drug interactions using the aforementioned SOPs. All data entry undergoes review by a second reviewer prior to public release.

Current Status of the Repository. An overview of data entered into the NaPDI Center repository is provided for two of the high-priority NPs selected as case studies: cannabis (*C. sativa*) and kratom (*M. speciosa*). These NPs were chosen due to increasing use and public interest. Neither NP has been well studied with respect to NPDI potential. In the United States, a majority of states have legalized marijuana for recreational and/or medical purposes. Moreover, a growing number of products containing the nonpsychotropic phytocannabinoid cannabidiol are marketed every year. These products include the FDA-approved drug Epidiolex and numerous unapproved tinctures, oils, and extracts. Kratom, a member of the coffee family native to Southeast Asia, is touted for its analgesic and stimulant effects. Warnings about kratom toxicity have been raised by the US FDA and the Centers for Disease Control and Prevention (Food and Drug Administration, 2019; Gershman, 2019). Calls to US poison centers involving kratom exposures from 2011 to 2017 increased 52-fold, from 13 to 682, with more than one-third of the calls reported involving co-consumption with prescription or illicit drugs (Post et al., 2019).

Each case study begins with a summary of NaPDI Center research activities focusing on each NP as a precipitant of pharmacokinetic NPDIs. A description follows about how published evidence was added to the repository to both complement the data generated by the NaPDI Center and provide researchers with a more complete picture of the pharmacokinetic interaction potential for each NP.

NPDI Study Process. Four steps are crucial for conducting a rigorous research study on a given pharmacokinetic NPDI: NP selection; sourcing and chemical characterization of different commercial products of the selected NP; in vitro assessment of inhibition or induction of drug metabolizing enzymes and

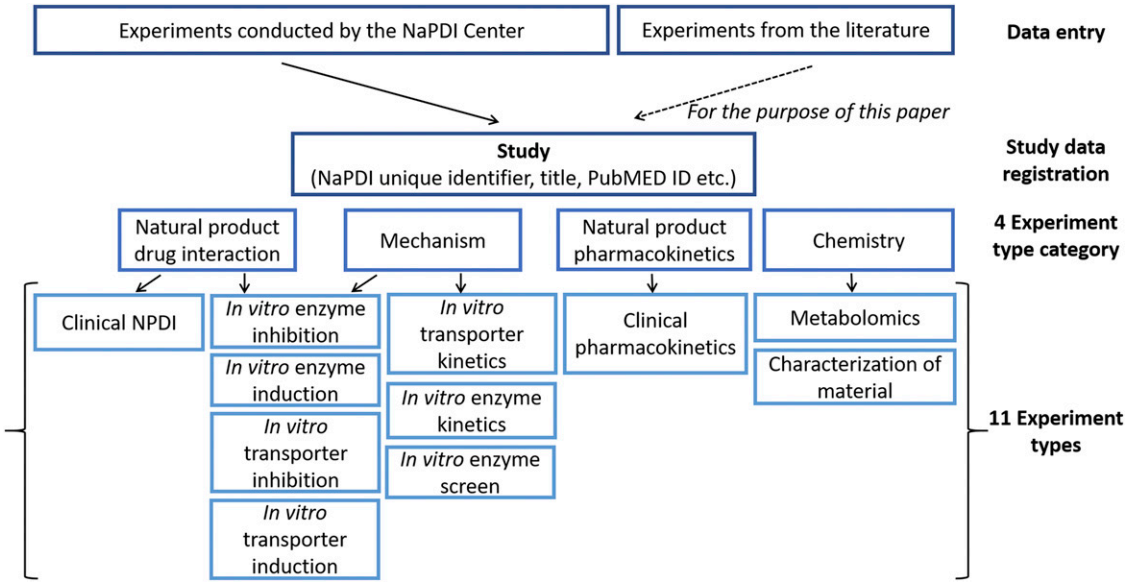

Fig. 2. Data resulting from experiments conducted by the NaPDI Center and from experiments reported in the literature are entered into the repository. Each "Study" record describes an activity that resulted in data from one or more related experiments. Each experiment record is assigned 1 of the 11 experiment types offered that provides the appropriate format for recording experimental conditions and results following instructions provided in the 11 SOPs.

TABLE 1

Data in the NaPDI Center repository are FAIR

FAIR	General
Findability	Each data set receives a unique identifier. Study and experiment metadata are published using a machine-readable format. The update frequency of the data is available for each study and experiment.
Accessibility	Full data sets are downloadable. Data are accessible in a variety of formats and can be retrieved using a REST-full API. The repository uses HTTP content negotiation to serve data requests. The repository search capabilities support simple search and advanced faceted search.
Interoperability	Data sets use data elements from existing ontologies and terminologies as much as possible. NMR and MS results are reported following accepted standards.
Reusability	Standard operating procedures are publicly available. Experiments are described in clear detail. Study and experiment metadata provide clear licensing requirements. Repository users can provide feedback and ask questions. Raw spectral data are available using an open file format.

API, application programming interface; HTTP, hypertext transfer protocol; MS, mass spectrometry; NMR, nuclear magnetic resonance; REST, representational state transfer.

transporters by the NP; and, if necessary based on the prior data, a clinical study of potential pharmacokinetic NPDIs in human subjects (Fig. 3).

The upper half of Figure 3 shows the cannabis studies conducted by the NaPDI Center as of March 2020. Chemical characterization data for two products were obtained from the National Center for Natural Products Research at the University of Mississippi. One product was an extract enriched in delta-9-tetrahydrocannabinol (THC) and the other was an extract enriched in cannabidiol (CBD). Purified THC and CBD were tested as inhibitors of five major cytochrome P450 (P450) enzymes, namely, CYP1A2, CYP2C9, CYP2C19, CYP2D6, and CYP3A4/5. Results informed the design of an ongoing clinical cannabis-drug interaction study.

The lower half of Figure 3 shows the kratom studies conducted by the NaPDI Center as of March 2020. The Analytical Core conducted a metabolomics study involving 55 kratom products, informing the selection of one product for further in vitro and clinical studies. The selection criteria followed a published NaPDI Center Recommended Approach (Kellogg et al., 2019). The Analytical Core conducted chemical characterization of the selected product to quantify mitragynine, 7-hydroxymitragynine, and speciofoline (Fig. 3). Extracts prepared from three kratom products, including one that was eventually selected for the clinical study, were tested by the Pharmacology Core as inhibitors of three major P450s, specifically CYP2C9, CYP2D6, and CYP3A4/5. As with cannabis, the in vitro results informed the design of the ongoing clinical kratom-drug interaction study.

Literature Search Process. Additional data were identified from peer-reviewed published reports in order for the data repository to provide greater research context for the NaPDI Center–conducted studies. Systematic literature searches were designed to retrieve studies on NP constituent pharmacokinetics and drug interactions involving either cannabis or kratom. The final search strategies are available in the Appendix. Queries were run in PubMed in July 2018 and again in February 2020.

The screening of titles and abstracts, and subsequently full text articles, was completed independently and in duplicate to identify experiments of the types shown in Figure 2. Mechanistic experiments of interest included assessing the NP as an inhibitor or inducer of P450s, UDP-glucuronosyltransferases (UGTs), and transporters. Clinical experiments of interest included pharmacokinetic NPDIs involving cannabis or kratom. Experiments involving only synthetic analogs, pharmacodynamics, or nonhuman animal studies and review articles were excluded. Full text articles available only in non-English languages were also excluded. Published reports cited in a recent review by the NaPDI Center (Cox et al., 2019) on cannabis pharmacology and pharmacokinetics ($n = 6$) were added to the screening results.

Data Entry of Published Literature and Pharmacokinetic NPDI Studies. Data from the included published reports were entered into the repository following the aforementioned SOPs (Boyce et al., 2020). When available, exact values from the text were entered. Otherwise, estimates were made from the study figures. Data extracted from each report were marked as "draft" during initial data entry and "pending" upon completion of data entry. After quality assurance by a second reviewer, the extracted data were made public. Data entry issues were tracked and addressed until quality assurance was complete for all studies.

Results

Construction and Content

As of April 2020, the NaPDI Center repository contains data from 777 experiments (Table 2). Currently, the most common experiment types are in vitro enzyme inhibition (405), in vitro enzyme induction (99), in vitro transport inhibition (78), and clinical pharmacokinetic NPDIs (57). The remaining 138 experiments are of various other types supported by the repository. In line with FAIR recommendations, every experiment is assigned a unique and persistent identifier that also resolves to a downloadable copy of a data set. A clear description of each experiment's conditions is provided by the repository website. The repository publishes metadata about each experiment that is machine readable and confirmed to work with Google's Dataset Search

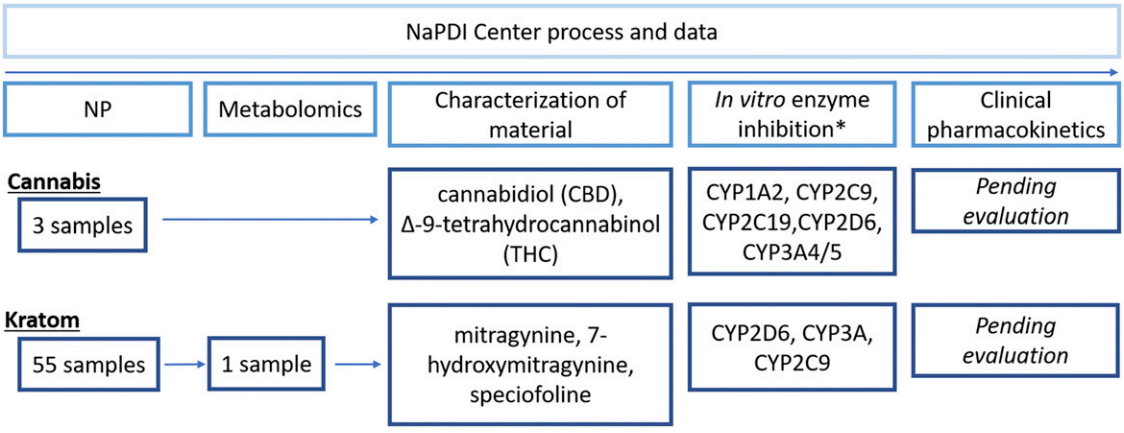

Fig. 3. Process and data undertaken by the NaPDI Center for the study of pharmacokinetic NPDIs precipitated by cannabis and kratom. *The Analytical Core did not source or characterize the cannabis study materials, whereas it conducted both investigations for kratom. The purified cannabis study materials were purchased from a commercial vendor.

TABLE 2

Number of experiments deposited in the NaPDI Center data repository as of April 2020 detailed for cannabis (*C. sativa*) and kratom (*M. speciosa*)

NaPDI Center repository (as of April 2020)	All high-priority NPs	Cannabis	Kratom
Chemical characterization experiments			
Characterization of NP study material	9	3	1
Metabolomics	3	0	1
In vitro experiments	99	5	61
Enzyme induction			
Enzyme inhibition	405	116	99
Enzyme kinetics	16	9	3
Enzyme screen	1	0	1
Transporter induction	55	13	32
Transporter inhibition	78	25	4
Transporter kinetics	34	2	10
Clinical NPDI experiments	57	33	0
Pharmacokinetic NPDI			
NP pharmacokinetics	20	7	0
Total	777	213	212

(https://datasetsearch.research.google.com/). To provide the most optimal experience to the researcher or editor wanting to search for data in the repository, an interactive and silent guided tour is provided on the home page (see the screen capture video in Supplemental Data).

Utility

This section reports the results of NaPDI Center repository data entry of the two high-priority NPs selected as case studies: cannabis (*C. sativa*) and kratom (*M. speciosa*).

Cannabinoids. Figure 4 provides an overview of reported NPDI data for cannabis from both NaPDI Center studies and peer-reviewed published reports. Links to the specific experiments are provided in Supplemental Table 2.

Chemical characterization data obtained from the National Center for Natural Products Research (https://pharmacy.olemiss.edu/ncnpr/) for two cannabis extracts and bulk plant material provided the exact concentration of CBD, THC, and other cannabinoids. The data confirmed the CBD-enriched extract (CBD 59.34%, THC 1.96%) to have a higher concentration of CBD than the bulk plant (CBD 0.04%, THC 11.7%) or THC-enriched extract (CBD 0%, THC 69.81%) (Fig. 4). NaPDI Center experiments confirmed that CBD inhibited CYP2C9, CYP3A4/5, CYP2C19, and CYP2D6 and that THC inhibited CYP2C9, CYP2C19, and CYP2D6 (unpublished data).

Data from a total of 22 published in vitro reports focusing on cannabis-drug interactions were entered into the repository (Holland et al., 2006, 2007, 2008; Zhu et al., 2006; Watanabe et al., 2007; Mazur et al., 2009; Alhamoruni et al., 2010; Tournier et al., 2010; Yamaori et al., 2010, 2011a,b, 2012, 2013, 2014, 2015; Jiang et al., 2011, 2013; Arnold et al., 2012; Al Saabi et al., 2013; Feinshtein et al., 2013a,b; Qian et al., 2019). As Figure 4 shows, experiments using either human liver microsomes or recombinant baculovirus–transfected insect cells expressing specific P450/UGT isoforms reported that cannabinoids inhibit CYP1A1, CYP1A2, CYP2C9, CYP2C19, CYP2D6, CYP3A4/5, and UGT (Mazur et al., 2009; Yamaori et al., 2010, 2011a,b, 2012, 2013; Al Saabi et al., 2013; Jiang et al., 2013; Qian et al., 2019). Yamaori et al. reported that CBD mechanistically inhibited CYP1A1 in vitro in recombinant baculovirus transfected insect cells. Qian et al. reported that CBD and cannabinol inhibited carboxylesterase 1 in vitro in human embryonic kidney 293 cells (Qian et al., 2019).

In vitro inhibition of P-glycoprotein–mediated efflux transport was reported for THC from experiments using transfected human embryonic kidney cells and for CBD using BeWo choriocarcinoma, LLC-PK1/MDR1, or MCF7/P-gp cells (Zhu et al., 2006; Tournier et al., 2010; Feinshtein et al., 2013a). An experiment using a human ovarian carcinoma cell line reported that cannabinol inhibited the efflux transporter multidrug resistance-associated protein 1 (MRP1 or ABCC1) (Holland et al., 2008). Experiments using BeWo, Jar, MCF7/P-gp, and MEF3.8/Bcrp A2 cell lines reported that CBD inhibited breast cancer resistance protein (BCRP or ABCG2), an effect that was reported for THC and cannabinol using the cell line MEF3.8/Bcrp A2 (Holland et al., 2008; Feinshtein et al., 2013b).

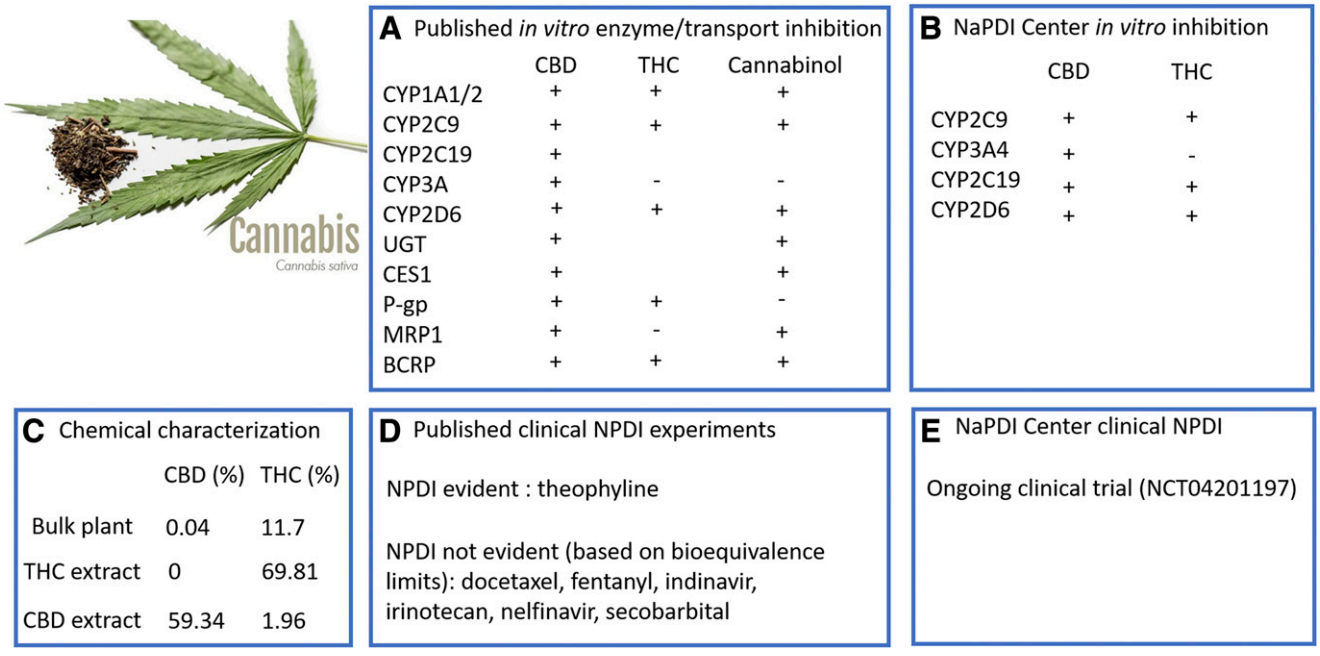

Fig. 4. Overview of reported NPDI data for cannabis from both NaPDI Center studies and peer-reviewed publications.

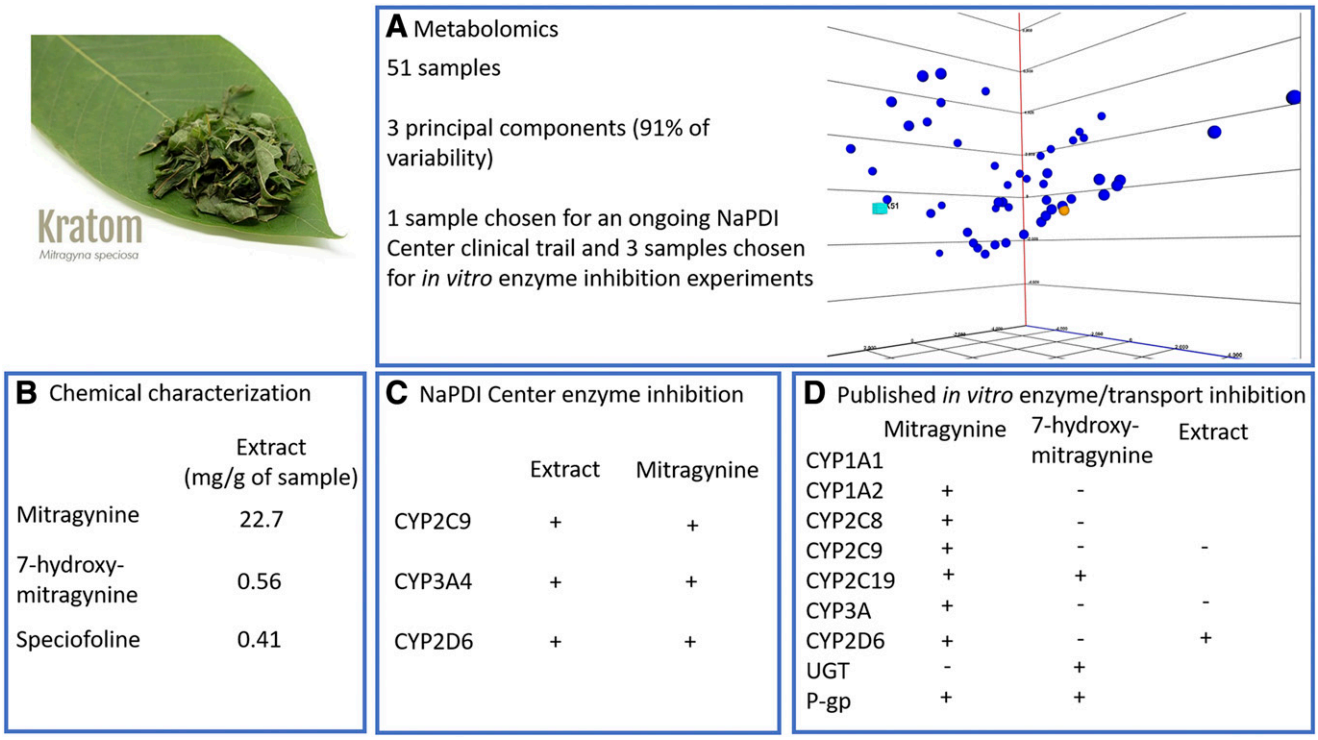

Fig. 5. Overview of reported NPDI data for kratom from both NaPDI Center studies and peer-reviewed publications. The results shown in boxes "b" and "c" are for the product chosen from the metabolomics study (light blue highlight in box "a").

A total of nine published clinical reports focusing on pharmacokinetic cannabis-drug interactions were entered into the repository (Dalton et al., 1976; Jusko et al., 1978; Perez-Reyes et al., 1988; Kosel et al., 2002; Haney et al., 2003; Engels et al., 2007; Kleinloog et al., 2012; Stott et al., 2013; Manini et al., 2015). Only one study reported an interaction involving smoked *C. sativa*, which was observed to increase the clearance of the CYP1A2 substrate theophylline (Jusko et al., 1978). Clinical pharmacokinetic interactions between cannabis and docetaxel, fentanyl, indinavir, irinotecan, nelfinavir, or secobarbital were not evident based on bioequivalence limits (Dalton et al., 1976; Kosel et al., 2002; Engels et al., 2007; Manini et al., 2015). One clinical study compared the plasma concentrations of THC and CBD under fasting and fed conditions (Stott et al., 2013), whereas another study reported estimated pharmacokinetic parameters for THC (Kleinloog et al., 2012).

Kratom. Figure 5 provides an overview of pharmacokinetic NPDI data for kratom from both NaPDI Center studies and peer-reviewed published reports. Links to the specific experiments are provided in Supplemental Table 3.

The Analytical Core's metabolomics analysis of 51 kratom products highlighted differences in chemical compound profiles depending on the manufacturer, form, and geographic location where the plants grew. A principal components analysis of the data identified three principal components explaining 91% of the variability across the features included in the metabolomics analysis.

Chemical characterization of the methanolic kratom extract used in the ongoing NaPDI in vitro and clinical studies (made from a clinical product) identified mitragynine (22.7 mg/g of sample), 7-hydroxymitragynine (0.57 mg/g of sample), and speciofoline (0.41 mg/g of sample). The in vitro inhibition studies showed that both the methanolic kratom extract and mitragynine inhibited CYP2C9, CYP2D6, and CYP3A4/5 by differing extents (unpublished observations).

Data from nine published in vitro studies were entered into the repository (Hanapi et al., 2010, 2013; Kong et al., 2011; Haron and Ismail, 2014; Manda et al., 2014; Meyer et al., 2015; Kamble et al., 2019, 2020; Rusli et al., 2019). One study using recombinant P450 enzymes reported that a methanolic extract of kratom inhibited CYP2D6 but not CYP2C9 or CYP3A4 (Hanapi et al., 2010). One study using pooled human liver microsomes reported inhibition of CYP2C19 by 7-hydroxymitragynine (Kamble et al., 2020), whereas another study using recombinant enzymes reported inhibition of UGT1A1 by 7-hydroxymitragynine (Haron and Ismail, 2014).

Mitragynine inhibition of CYP2D6 was reported in three different studies using pooled human liver microsomes (Kamble et al., 2020), recombinant P450s (Hanapi et al., 2013), and a high-throughput in vitro fluorescent P450 assay (Kong et al., 2011). Mitragynine inhibition of CYP3A and CYP2C19 was reported with pooled human liver microsomes (Kamble et al., 2020) and the in vitro fluorescent P450 assay (Kong et al., 2011). Mitragynine inhibition of CYP2C8 was reported with pooled human liver microsomes (Kamble et al., 2020), CYP1A2 with an in vitro fluorescent P450 assay (Kong et al., 2011), and CYP2C9 with recombinant P450 enzymes (Hanapi et al., 2013).

Three studies reported inhibition of P-glycoprotein by mitragynine, two using Caco-2 cells (Meyer et al., 2015; Rusli et al., 2019), and one using MDCK-transfected cells (Manda et al., 2014). The same MDCK-transfected cell study reported inhibition of P-glycoprotein by 7-hydroxymitragynine. One study reported CYP3A4 as the primary metabolizing enzyme for mitragynine (Kamble et al., 2019). Another study reported downregulation of P-glycoprotein in Caco-2 cells by mitragynine (Rusli et al., 2019).

Discussion

Although rigorous pharmacokinetic NPDI research can mitigate adverse interactions, the data and knowledge resulting from these experiments are currently distributed across a variety of information sources, making them difficult to find, access, and reuse. The new

NaPDI Center repository is the first user-friendly online repository that stores and links pharmacokinetic NPDI data across chemical characterization, metabolomics analyses, and pharmacokinetic in vitro and clinical experiments. The design is expected to help researchers more easily arrive at a complete understanding of pharmacokinetic NPDI research on a particular NP. The repository will also facilitate multidisciplinary collaborations, as the repository links all of the experimental data for a given NP across the study types. For example, the repository links chemical characterization data with data from in vitro and clinical experiments and vice versa. This feature should help facilitate communication between multidisciplinary researchers working on different aspects of a particular pharmacokinetic NPDI.

The mission of the NaPDI Center is to provide leadership and guidance on the study of pharmacokinetic NPDIs. Currently, only data on the four high-priority NPs under study by the NaPDI Center have been entered in the repository. Future work hopes to expand the repository to include a larger selection of NPs and engage NPDI researchers external to the NaPDI Center. Toward that goal, pilot work is completed that includes data from experiments involving P450 inhibition by three licorice species (i.e., *Glycyrrhiza glabra*, *G. uralensis*, and *G. inflata*) (Li et al., 2017). The published report includes pharmacokinetic NPDI data specific to extracts of each licorice species and for individual constituents present in some or all licorice species. The repository links all of these data in a manner that allows researchers to explore P450 inhibition by licorice from a variety of perspectives (i.e., single or multiple licorice species and single or multiple licorice constituents). It is useful to emphasize that the NaPDI Center repository currently focuses on pharmacokinetic NPDI data. At the present time there are no plans to integrate pharmacodynamic NPDI data. Though it has not been the focus to date, the format for data in the NaPDI data repository allows for setting the NP as the object drug, and there are a handful of experiments in the repository of this kind that have been entered as test cases. The inclusion of this kind of data might become the focus in the future depending on feedback from the NPDI research community and other stakeholders.

Building upon this strong foundation, the NaPDI Center plans to create novel information visualizations to provide researchers a complete evidence-based overview of the potential of each NP to precipitate pharmacokinetic NPDIs. The Center also plans to permit other researchers to submit data using files or the repository's web-based application programming interface with the goal of supporting medium- to high-throughput assays that generate megabytes or gigabytes of data. Researchers external to the NaPDI Center can enter data by first requesting an account and then following the SOP documents during data entry. After a researcher's data entry is completed, a trained individual within the NaPDI Center will inspect the entered data before public release.

Finally, the NaPDI Center plans to implement automatic FAIR quality analytic reports that will run each time a data submitter marks a new study entry as "pending." Issues identified from the reports can then be addressed promptly by the data submitter. These functionalities, combined with the existing functionalities of the NaPDI Center repository, seek to facilitate pharmacokinetic NPDI research with the long-range goal of mitigating adverse interactions and improving public health.

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Authorship Contributions

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Wrote or contributed to the writing of the manuscript: Birer-Williams, Gufford, Alilio, VanAlstine, Morley, McCune, Paine, Boyce.

Appendix: Search Strategy for Cannabis

Clinical Studies

(Clinical Trial [PT] AND (Cannabis[MeSH Terms] OR "cannabinoids"[All Fields] OR "Cannabidiol"[All Fields] OR "CBD"[All Fields] OR "Cannabinol"[All Fields] OR "Dronabinol"[All Fields] OR "delta(9)-THC"[All Fields] OR "9-ene-Tetrahydrocannabinol"[All Fields] OR "9 ene Tetrahydrocannabinol"[All Fields] OR "THC"[All Fields] OR "delta(1)-Tetrahydrocannabinol"[All Fields] OR "delta(1)-THC"[All Fields] OR "delta(9)-Tetrahydrocannabinol"[All Fields] OR "Tetrahydrocannabinol"[All Fields] OR "Tetrahydrocannabinol, (6a-trans)-Isomer"[All Fields] OR "Tetrahydrocannabinol, Trans-Isomer"[-All Fields] OR "Tetrahydrocannabinol, Trans Isomer"[All Fields] OR "Tetrahydrocannabinol, (6aS-cis)-Isomer"[All Fields] OR "Tetrahydrocannabinol, Trans-(+-)-Isomer"[All Fields] OR "Marinol"[All Fields] OR "Tetrahydrocannabinol, (6aR-cis)-Isomer"[All Fields] OR "delta-9-tetrahydrocannabinol"[All Fields] OR "(-)delta-9-tetrahydrocannabinol"[All Fields] OR "THC"[All Fields]) AND "drug interactions"[All Fields]) NOT Review [PT].

Mechanistic NPDI studies useful for inferring NPDIs:

Step 1) Log into My NCBI and go to Pubmed: https://www.ncbi.nlm.nih.gov/pubmed/.

Step 2) In the advanced search form, clear the search history.

Step 3) Paste in this query into builder (using "edit") and click "add to history"—this step is referred to as "#1" in the rest of this search strategy:

"Cytochrome P-450 Enzyme System"[MeSH Terms] OR "Cytochrome P450 Family 1"[MeSH Terms] OR "Cytochrome P450 Family 2"[MeSH Terms] OR "Cytochrome P450 Family 3"[MeSH Terms] OR CYP1A1[All Fields] OR CYP1A2[All Fields] OR CYP1A3[All Fields] OR CYP1A4[All Fields] OR CYP1A5[All Fields] OR CYP2D6[All Fields] OR CYP2C9[All Fields] OR CYP2A6[All Fields] OR CYP2C8 [All Fields] OR CYP2C19[All Fields] OR CYP2B6[All Fields] OR CYP2B1[All Fields] OR CYP2E1[All Fields] OR CYP3A4[All Fields] OR CYP3A5[All Fields] OR UGT1[All Fields] OR UGT1A1[All Fields] OR UGT1A3[All Fields] OR UGT1A4[All Fields] OR UGT1A5[All Fields] OR UGT1A6[All Fields] OR UGT1A7[All Fields] OR UGT1A8[All Fields] OR UGT1A9[All Fields] OR UGT1A10[All Fields] OR UGT2[All Fields] OR UGT2A1[All Fields] OR UGT2A2 [All Fields] OR UGT2A3[All Fields] OR UGT2B4[All Fields] OR UGT2B7[All Fields] OR UGT2B10[All Fields] OR UGT2B11[All Fields] OR UGT2B15[All Fields] OR UGT2B17[All Fields] OR UGT2B28[All Fields] OR B3GAT1[All Fields] OR B3GAT2[All Fields] OR B3GAT3[All Fields].

Step 4) Paste in this query into builder (using "edit") and click "add to history"—this is referred to as "#2" in the rest of this search strategy.

"Solute Carrier Proteins"[MeSH Terms] OR "Membrane Transport Proteins"[MeSH Terms] OR "P-gp"[All Fields] OR "p-glycoprotein"[All Fields] OR BCRP[All Fields] OR OCT2[All Fields] OR

"Organic Cation Transporter 2"[MeSH Terms] OR "Organic Cation Transport Proteins"[MeSH Terms] OR MATE1[All Fields] OR "SLC4A Proteins"[MeSH Terms] OR MATE-2K[All Fields] OR "SLC4A Proteins"[MeSH Terms] OR OATP[All Fields] OR OAT1 [All Fields] OR "Organic Anion Transport Protein 1"[MeSH Terms] OR OAT3[All Fields] OR UGT1[All Fields] OR "Glucuronosyltransferase"[MeSH Terms] OR ABC[All Fields] OR "ATP-Binding Cassette Transporters"[MeSH Terms]

Step 5) Paste in this query into builder (using "edit") and click "add to history"—this step is referred to as "#3" in the rest of this search strategy.

(Cannabis[MeSH Terms] OR "cannabinoids"[All Fields] OR "Cannabidiol"[All Fields] OR "CBD"[All Fields] OR "Cannabinol"[All Fields] OR "Dronabinol"[All Fields] OR "delta(9)-THC"[All Fields] OR "9-ene-Tetrahydrocannabinol"[All Fields] OR "9 ene Tetrahydrocannabinol"[All Fields] OR "THC"[All Fields] OR "delta(1)-Tetrahydrocannabinol"[All Fields] OR "delta(1)-THC"[All Fields] OR "delta(9)-Tetrahydrocannabinol"[All Fields] OR "Tetrahydrocannabinol"[All Fields] OR "Tetrahydrocannabinol, (6a-trans)-Isomer"[All Fields] OR "Tetrahydrocannabinol, Trans-Isomer"[All Fields] OR "Tetrahydrocannabinol, Trans Isomer"[All Fields] OR "Tetrahydrocannabinol, (6aS-cis)-Isomer"[All Fields] OR "Tetrahydrocannabinol, Trans-(+-)-Isomer"[All Fields] OR "Marinol"[All Fields] OR "Tetrahydrocannabinol, (6aR-cis)-Isomer"[All Fields] OR "delta-9-tetrahydrocannabinol"[All Fields] OR "(-)delta-9-tetrahydrocannabinol"[All Fields] OR "THC"[All Fields]).

Step 6) Paste in this query into builder (using "edit") and click "add to history"—this is referred to as "#4" in the rest of this search strategy.

(Pharmacokinetics[MeSH Terms] OR pharmacokinetic[All Fields]) or (inhibit[All Fields] or inhibition[All Fields]) OR substrate[All Fields]

Step 7) Paste in this query into builder (using "edit") and click "add to history"—this step is referred to as "#5" in the rest of this search strategy.

#3 AND #4 AND (#1 OR #2) AND "humans"[MeSH Terms].

Search Strategy for Kratom

Clinical Studies

(Clinical Trial [PT] AND ("mitragynine"[All Fields] OR "mitragynine ethanedisulfonate"[All Fields] OR "SK and F 12711"[All Fields] OR "SKF 12711"[All Fields] OR "SK and F-12711"[All Fields] OR "mitragynine, (16E)-isomer"[All Fields] OR "mitragynine, (3beta,16E)-isomer"[All Fields] OR "mmitragynine, (3beta,16E,20beta)-isomer"[All Fields] OR "kratom alkaloids"[All Fields] OR "kmitragynine monohydrochloride"[All Fields] OR "Mitragyna speciosa"[All Fields] OR "Nauclea speciose"[All Fields] OR "Biak-biak"[All Fields] OR "Cratom"[All Fields] OR "Gratom"[All Fields] OR "Ithang"[All Fields] OR "Kakuam"[All Fields] OR "Katawn"[All Fields] OR "Kedemba"[All Fields] OR "Ketum"[All Fields] OR "Krathom"[All Fields] OR "Kraton"[All Fields] OR "Kratum"[All Fields] OR "Madat"[All Fields] OR "Mambog"[All Fields] OR "Mitragynine"[All Fields] OR "Mitragynine extract"[All Fields] OR "Thang"[All Fields] OR "Thom"[All Fields] OR "7-hydroxymitragynine"[All Fields] OR "7-hydroxy-mitragynine"[All Fields] OR "mitragynine pseudoindoxyl"[All Fields] OR "Paynantheine"[All Fields]) AND "drug interactions"[All Fields]) NOT Review [PT]

Mechanistic NPDI studies useful for inferring NPDIs:

Step 1) Log into My NCBI and go to Pubmed: https://www.ncbi.nlm.nih.gov/pubmed/.

Step 2) In the advanced search form, clear the search history.

Step 3) Paste in this query into builder (using "edit") and click "add to history"—this is referred to as "#1" in the rest of this search strategy:

"Cytochrome P-450 Enzyme System"[MeSH Terms] OR "Cytochrome P450 Family 1"[MeSH Terms] OR "Cytochrome P450 Family 2"[MeSH Terms] OR "Cytochrome P450 Family 3"[MeSH Terms] OR CYP1A1[All Fields] OR CYP1A2[All Fields] OR CYP1A3[All Fields] OR CYP1A4[All Fields] OR CYP1A5[All Fields] OR CYP2D6[All Fields] OR CYP2C9[All Fields] OR CYP2A6[All Fields] OR CYP2C8 [All Fields] OR CYP2C19[All Fields] OR CYP2B6[All Fields] OR CYP2B1[All Fields] OR CYP2E1[All Fields] OR CYP3A4[All Fields] OR CYP3A5[All Fields] OR UGT1[All Fields] OR UGT1A1[All Fields] OR UGT1A3[All Fields] OR UGT1A4[All Fields] OR UGT1A5[All Fields] OR UGT1A6[All Fields] OR UGT1A7[All Fields] OR UGT1A8[All Fields] OR UGT1A9[All Fields] OR UGT1A10[All Fields] OR UGT2[All Fields] OR UGT2A1[All Fields] OR UGT2A2 [All Fields] OR UGT2A3[All Fields] OR UGT2B4[All Fields] OR UGT2B7[All Fields] OR UGT2B10[All Fields] OR UGT2B11[All Fields] OR UGT2B15[All Fields] OR UGT2B17[All Fields] OR UGT2B28[All Fields] OR B3GAT1[All Fields] OR B3GAT2[All Fields] OR B3GAT3[All Fields].

Step 4) Paste in this query into builder (using "edit") and click "add to history"—this is referred to as "#2" in the rest of this search strategy.

"Solute Carrier Proteins"[MeSH Terms] OR "Membrane Transport Proteins"[MeSH Terms] OR "P-gp"[All Fields] OR "p-glycoprotein"[All Fields] OR BCRP[All Fields] OR OCT2[All Fields] OR "Organic Cation Transporter 2"[MeSH Terms] OR "Organic Cation Transport Proteins"[MeSH Terms] OR MATE1[All Fields] OR "SLC4A Proteins"[MeSH Terms] OR MATE-2K[All Fields] OR "SLC4A Proteins"[MeSH Terms] OR OATP[All Fields] OR OAT1 [All Fields] OR "Organic Anion Transport Protein 1"[MeSH Terms] OR OAT3[All Fields] OR UGT1[All Fields] OR "Glucuronosyltransferase"[MeSH Terms] OR ABC[All Fields] OR "ATP-Binding Cassette Transporters"[MeSH Terms].

Step 5) Paste in this query into builder (using "edit") and click "add to history"—this is referred to as "#3" in the rest of this search strategy.

("mitragynine"[All Fields] OR "mitragynine ethanedisulfonate"[All Fields] OR "SK and F 12711"[All Fields] OR "SKF 12711"[All Fields] OR "SK and F-12711"[All Fields] OR "mitragynine, (16E)-isomer"[All Fields] OR "mitragynine, (3beta,16E)-isomer"[All Fields] OR "mmitragynine, (3beta,16E,20beta)-isomer"[All Fields] OR "kratom alkaloids"[All Fields] OR "kmitragynine monohydrochloride"[All Fields] OR "Mitragyna speciosa"[All Fields] OR "Nauclea speciose"[All Fields] OR "Biak-biak"[All Fields] OR "Cratom"[All Fields] OR "Gratom"[All Fields] OR "Ithang"[All Fields] OR "Kakuam"[All Fields] OR "Katawn"[All Fields] OR "Kedemba"[All Fields] OR "Ketum"[All Fields] OR "Krathom"[All Fields] OR "Kraton"[All Fields] OR "Kratum"[All Fields] OR "Madat"[All Fields] OR "Mambog"[All Fields] OR "Mitragynine"[All Fields] OR "Mitragynine extract"[All Fields] OR "Thang"[All Fields] OR "Thom"[All Fields] OR "7-hydroxymitragynine"[All Fields] OR "7-hydroxy-mitragynine"[All Fields] OR "mitragynine pseudoindoxyl"[All Fields] OR "Paynantheine"[All Fields]).

Step 6) Paste in this query into builder (using "edit") and click "add to history"—this is referred to as "#4" in the rest of this search strategy.

(Pharmacokinetics[MeSH Terms] OR pharmacokinetic[All Fields]) or (inhibit[All Fields] or inhibition[All Fields]) OR substrate[All Fields].

Step 7) Paste in this query into builder (using "edit") and click "add to history"—this is referred to as "#5" in the rest of this search strategy.

#3 AND #4 AND (#1 OR #2) AND "humans"[MeSH Terms].

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Zhu H-J, Wang J-S, Markowitz JS, Donovan JL, Gibson BB, Gefroh HA, and Devane CL (2006) Characterization of P-glycoprotein inhibition by major cannabinoids from marijuana. *J Pharmacol Exp Ther* **317**:850–857.

Address correspondence to: Dr. Richard D. Boyce, University of Pittsburgh, The Offices at Baum, Suite 419, 5607 Baum Blvd, Pittsburgh, PA 15206. E-mail: rdb20@pitt.edu

NaPDI Repository Data Entry SOP: In vitro Enzyme Inhibition Studies

Version 1

Creation Date: March 2017

Author: Jessica Tay-Sontheimer

NOTE: This version is provided as supplemental information for a manuscript. Please check the github repository for this project as any more recent version on github supercedes this version:

https://github.com/dbmi-pitt/NaPDI-SOPs

Contents

1 BACKGROUND

1.1 SCOPE

The purpose of this Standard Operating Procedure (SOP) is to describe how to enter *in vitro* enzyme inhibition results into the NaPDI repository. Natural Products (NPs) are expected to be evaluated as causative agents of inhibition (*Precipitants*). The victim drugs (*Objects*) are probe substrates of known enzymes.

Most of the information entered in the repository will come directly from the study report; avoid interpretations of the authors' conclusions. However, several text fields are provided throughout the admin site to allow the addition of relevant comments that may pertain to the experimental study design and conditions, the study results, and/or the mechanism of inhibition. This additional information should be reviewed with the principal investigators during the validation process as it will be used to enrich the users experience and understanding of the results.

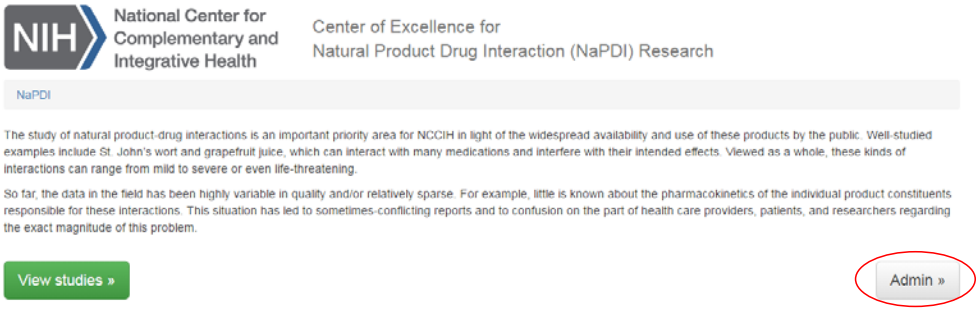
1.2 DEFINITIONS

Add user-centered definitions (alphabetically)

2 CREATING A STUDY

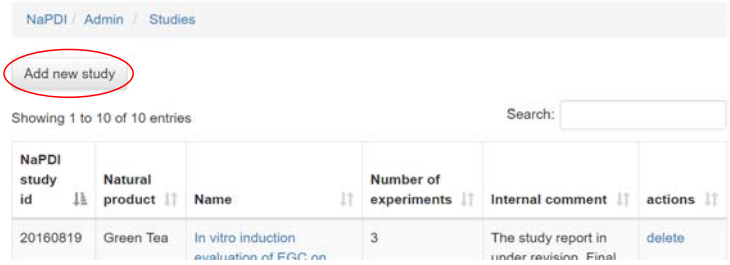
Use the following steps to create a new study.

2.1 Navigate to the Admin page of the NaPDI Repository



2.2 Using the admin page, click on "Studies"

2.3 then, click on “Add new study”



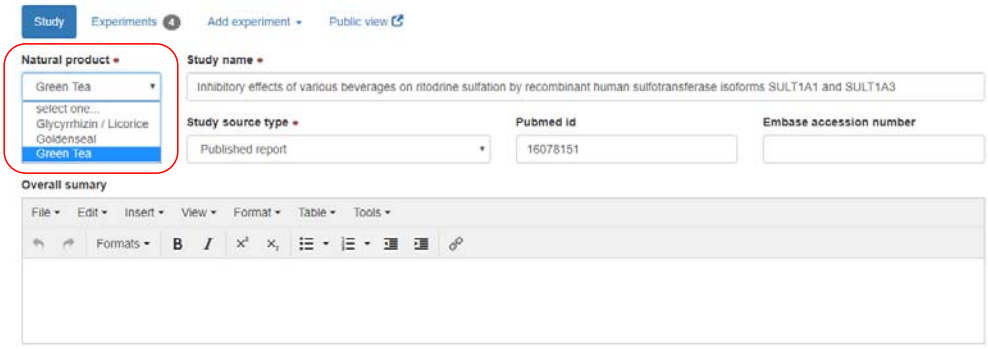
3 STUDY PAGE

A study can only accept data from one Natural Product and one species. For example, *in vitro* data with Licorice *Glycyrrhiza glabra* L., *Glycyrrhiza uralensis* Fish have to be reported in two different studies, one for each Licorice species.

3.1 Select the **Natural Product** tested in the *in vitro* study from the drop down list provided (select one; required):

- Licorice
- Goldenseal
- Green Tea

3.2 From the Study Report, enter the **Study Name** and **NaPDI Study ID** (required, as presented in Study Report).



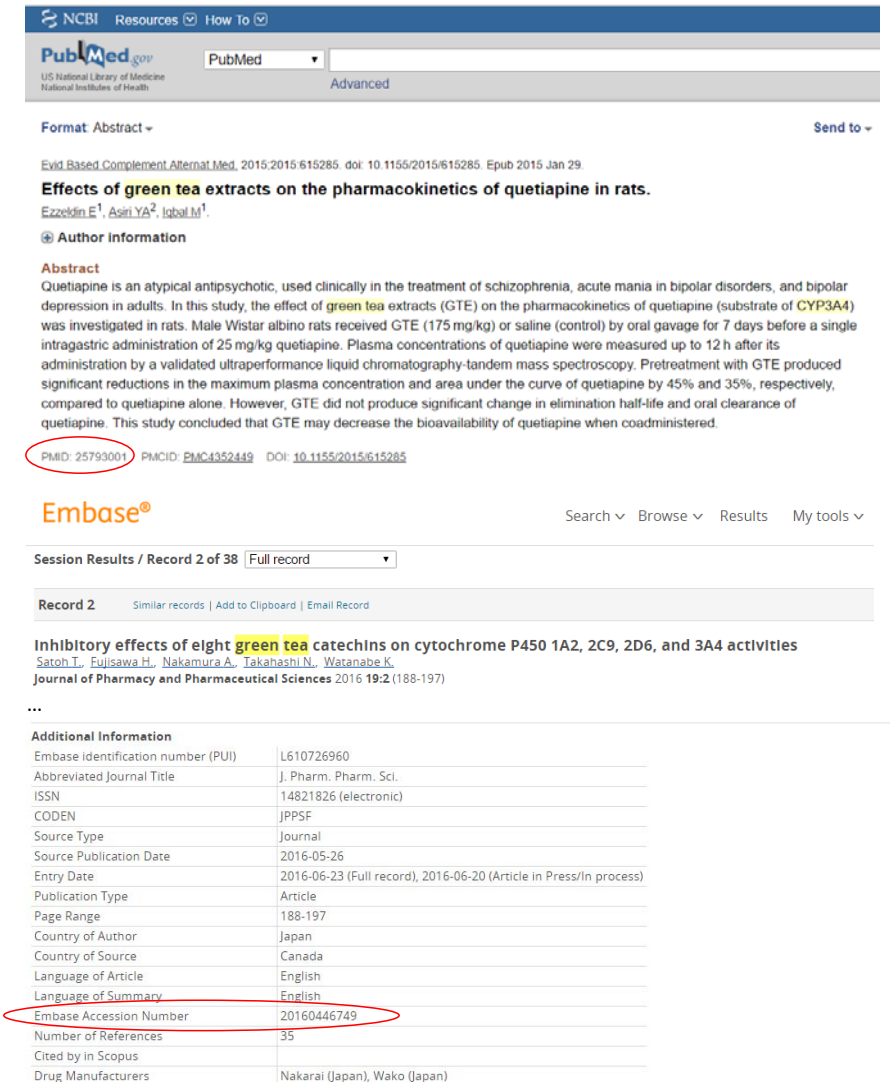
If a entries originate from a published paper, used the Pubmed ID or Embase PUI as the NaPDI Study ID (e.g., "PMID:23268924")

3.3 Select the **study source type** or source from which the study was obtained (required).

- Published report
- Manuscript prepared or submitted for peer-reviewed publication
- Unpublished data submitted through a NaPDI form

3.4 When a study has been published, enter the **PubMed ID** and/or **Embase Accession** number(s) (optional).

Tip: If the PubMed ID or Embase Accession number(s) cannot be located in the Study Report, they can be found under the abstract in PubMed or in the "Additional Information" section when the article's full record is viewed in Embase.



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Evid Based Complement Alternat Med. 2015;2015:615285. doi: 10.1155/2015/615285. Epub 2015 Jan 29.

Effects of green tea extracts on the pharmacokinetics of quetiapine in rats.

Ezzeldin E[1], Asiri YA[2], Iqbal M[1].

Author information

Abstract

Quetiapine is an atypical antipsychotic, used clinically in the treatment of schizophrenia, acute mania in bipolar disorders, and bipolar depression in adults. In this study, the effect of green tea extracts (GTE) on the pharmacokinetics of quetiapine (substrate of CYP3A4) was investigated in rats. Male Wistar albino rats received GTE (175 mg/kg) or saline (control) by oral gavage for 7 days before a single intragastric administration of 25 mg/kg quetiapine. Plasma concentrations of quetiapine were measured up to 12 h after its administration by a validated ultraperformance liquid chromatography-tandem mass spectroscopy. Pretreatment with GTE produced significant reductions in the maximum plasma concentration and area under the curve of quetiapine by 45% and 35%, respectively, compared to quetiapine alone. However, GTE did not produce significant change in elimination half-life and oral clearance of quetiapine. This study concluded that GTE may decrease the bioavailability of quetiapine when coadministered.

PMID: 25793001 PMCID: PMC4352449 DOI: 10.1155/2015/615285

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Record 2 Similar records | Add to Clipboard | Email Record

Inhibitory effects of eight green tea catechins on cytochrome P450 1A2, 2C9, 2D6, and 3A4 activities

Satoh T., Fujisawa H., Nakamura A., Takahashi N., Watanabe K.

Journal of Pharmacy and Pharmaceutical Sciences 2016 **19:2** (188-197)

...

Additional Information

Embase identification number (PUI)	L610726960
Abbreviated Journal Title	J. Pharm. Pharm. Sci.
ISSN	14821826 (electronic)
CODEN	JPPSF
Source Type	Journal
Source Publication Date	2016-05-26
Entry Date	2016-06-23 (Full record), 2016-06-20 (Article in Press/In process)
Publication Type	Article
Page Range	188-197
Country of Author	Japan
Country of Source	Canada
Language of Article	English
Language of Summary	English
Embase Accession Number	20160446749
Number of References	35
Cited by in Scopus	
Drug Manufacturers	Nakarai (Japan), Wako (Japan)

3.4 **Overall summary**: this summary should provide a concise overall conclusion of the *in vitro* study and also discuss the possible mechanism(s) involved (optional).

Comment [RDB1]: How many words? Studies can consist of numerous experiments. Please provide some example statements so that the scope of this comment field is more clear.

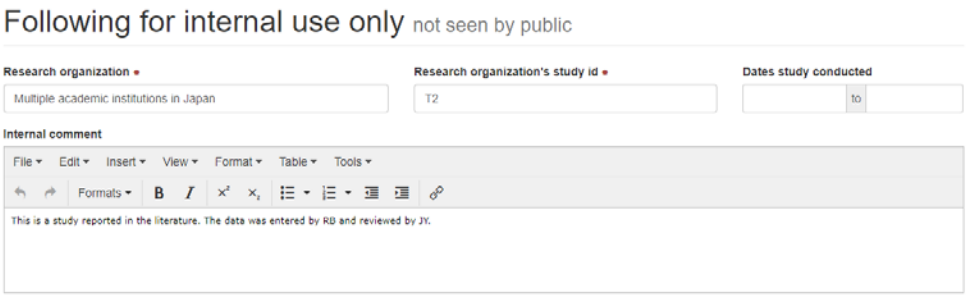
If entries are from a published paper, copy and paste the abstract into the Overall summary box.

3.5 The **Following for internal use only** section is designated for internal notes and will not be displayed to users.

3.5.1 Enter the **Research organization** name (where the study was performed) and their **study ID number** in the internal use section displayed below (required).

3.5.2 From the Study Report, enter the **dates the study was conducted** (optional). If only months are provided, select the first and last days of the month for the starting and ending date, respectively. For example, March to April, 2017 will be entered as 03/01/2017 to 04/30/2017.

3.5.3 Enter **internal comments** associated with the study that are intended for internal use only (optional).



3.6 Select the status of the current study entry

- Draft – selected when the curator is in the process of entering the data or checking the data
- Pending review – selected when the study had been fully entered by the curator and needs to be reviewed and validated by a second editor
- Published – selected after validation and is ready for public display

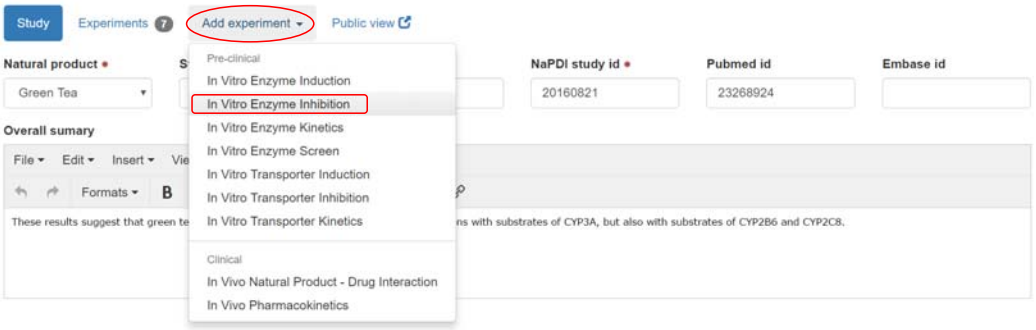
Comment [JS2]: Tell chris that a non-unique ID triggers an error.

Comment [RDB3]: Please refer to a specific reference that these ids will come from.

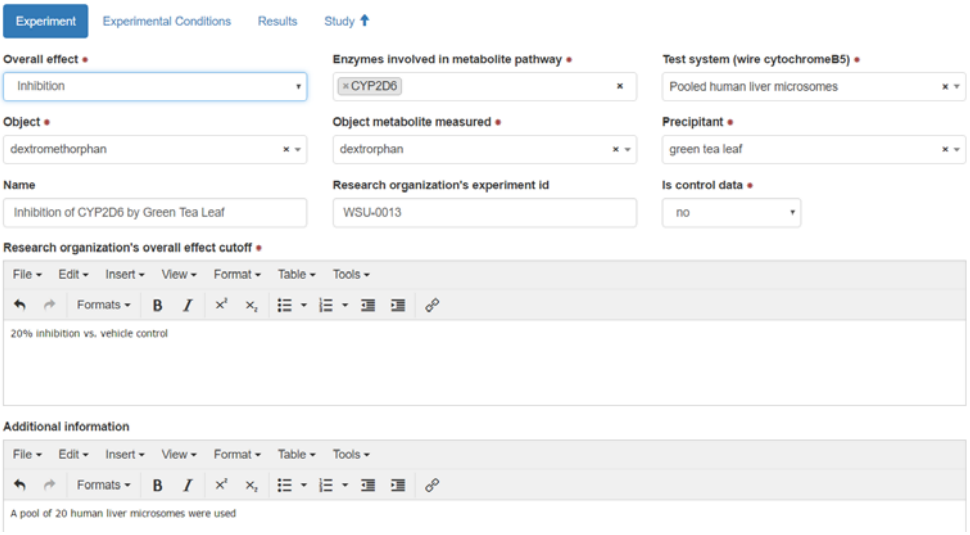
4 EXPERIMENT

After a study has been created, use the following steps to add a new experiment. Add a new experiment for determinations of parameters having a distinct set of experimental conditions from previous experiments (i.e., different object concentrations, different inhibitor concentrations, etc.).

4.1 Click on **add experiment**, then select **In Vitro Enzyme Inhibition** from the drop-down menu.



4.2 Select the **Overall effect**: "Inhibition", or "Negligible Inhibition" of the metabolism of the *Object,* based on study findings stated in the Study Report (select one; required). Use the authors' conclusions to make this determination. For example, if inhibition was observed, but the authors concluded no effect because it was not statistically significant, then "Negligible Inhibition" should be selected. Conversely, if 19% inhibition was observed with a 20% cut-off and the authors concluded weak inhibition, then "Inhibition" should be selected.



4.3 Select the **Enzyme(s) involved in the metabolite pathway** as stated in the Study Report (select many; required). Multiple selections can be made; therefore, select all enzymes responsible for the formation of the metabolite (if specific formation of metabolite is measured) or parent disappearance (if parent disappearance is measured).

Notes:

(1) When an enzyme studied is not listed in the drop-down menu, add the enzyme or state the enzyme in the **Additional information** section (see below).

(2) When variant enzymes are studied, select the variant enzyme and specify the variant in the **Additional information** text box (see below).

4.4 Select the *in vitro* **test system** used (select one; required).

Notes:

(1) For **recombinant expression systems** only, appropriately select **Cytochrome b5** conditions.

Choose:

- "Yes, co-expressed" if Cytochrome b5 was used and co-expressed in the recombinant system
- "Yes, supplemented" if Cytochrome b5 was used and was added to the incubation
- "No" if Cytochrome b5 was not used
- "Not available" if conditions regarding Cytochrome b5 are not provided in the Study Report

(2) If a study used a few donors of human liver microsomes, but each donor was evaluated individually, and results were presented as the mean value from all the donors, select

"pooled" source and add a comment stating that experiments were conducted in HLMs from individual donors in the **Additional information** section.

4.5 Select the **Object** and **Object metabolite** measured from the compound lists (select one; required). If the compound is not listed, add the compound. Enter only the study vehicle control (i.e. not the positive or negative control) as the object. Enter the details regarding the positive/negative control in the Additional Information section under this tab.

4.6 Select the **Precipitant** from the compound list (select one; required). If the compound is not listed, add the compound.

4.7 Enter an experiment **Name**, if provided (optional). Use title case, where the first word and all major words are capitalized (i.e., "Inhibition of CYP2D6 by Green Tea Leaf", NOT "Inhibition of CYP2D6 by green tea leaf".) Experiment names are used as sub-headings in the public view; therefore, names that describe the enzyme(s) involved in the pathway of the metabolite and the precipitant used in the study are best suited for this purpose.

4.8 If provided, enter the **research organization's experiment identification number** for this experiment only (optional).

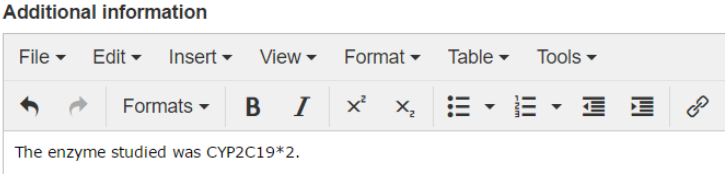
4.9 If this data corresponds to the control experiment for the study, choose "yes" from the **Is control data** drop-down menu (select one; required). Otherwise, choose "no". The "Is control data" function allows experiments to be linked within the repository. It only appears on the admin side and not in the public view.

4.10 Enter the **Research organization's overall effect cutoff** (required) described in the Study Report (for example, "20% inhibition versus control"). Enter multiple cut-offs if more than one is provided in the Study Report. If the authors did not provide this, attempts should be made to obtain this information. Enter "not applicable" when the cut-off is not applicable.
For published reports, enter "not available" or "N/A" when this information is not available or not applicable.

4.11 Enter **Additional information** important to the overall study, but where the details were not included in the fields above (optional). Enter only the study vehicle control (i.e. not the positive or negative control) as the object. Enter the details regarding the positive/negative control in the Additional Information section under this tab.

For example:

- variant enzymes, other enzymes or test systems not listed in the drop-down menu



- variations on the precipitant selected

Goldenseal flower bud methanol extract was used.

- results of other experiments used to determine the enzyme(s) involved in the formation of the metabolite

The enzymes responsible for the formation of the metabolite were identified through phenotyping studies.

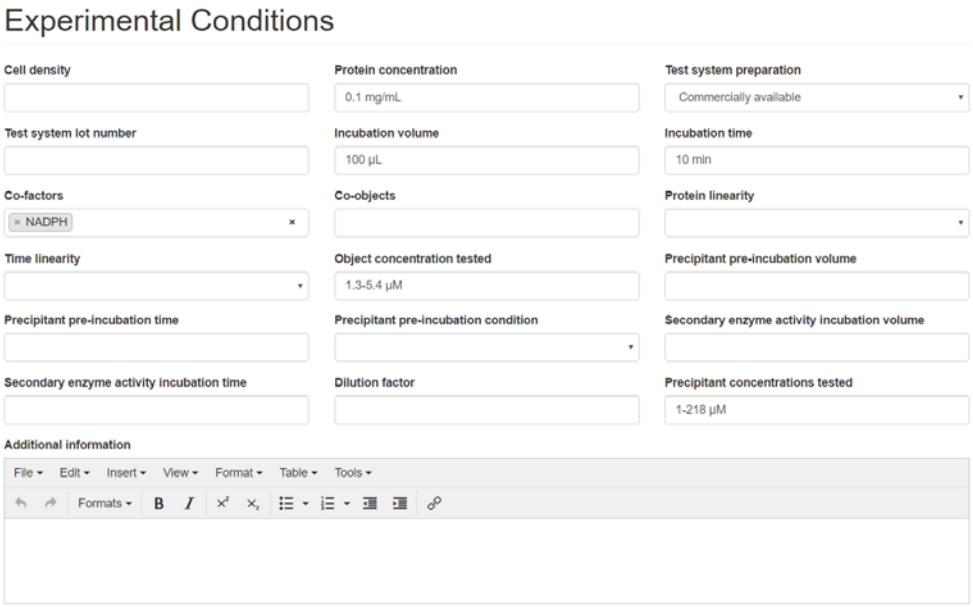
Comment [RDB4]: It will be REALLY helpful if folks can save as they complete each section, or just anytime at all. In fact, these days, people are used to data being saved as they type it in. Rather than 'submit' or 'save; one could 'validate' or 'finalize submission' or similar.

5 EXPERIMENTAL CONDITIONS

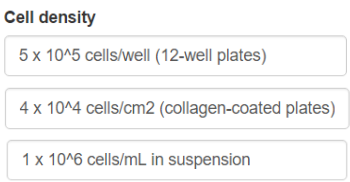
Enter experimental details that are provided in the Study Report.

Note that in many cases, some of the provided fields may be left blank.

> When entering conditions from published literature that refer to experimental conditions described in a reference, check the reference for conditions that are not clearly stated in the article. For example, if an article states that CYP1A2 substrates and concentrations used in Vivid CYP screening assays were used as described in Cheng et al. and the authors do not describe any further details, check Cheng et al. for experimental conditions and enter those stated therein. Also, make a comment in the additional information section regarding which parameters were extracted from the reference citation (*e.g.*, Object and object concentrations tested were extracted from Cheng et al., 2017).



5.1 Cell density: Enter the cell density in scientific notation. Specify the units and the type of culture plates or dishes used (optional). Examples are shown below:



5.2 **Protein concentration:** Enter the total protein concentration and specify the units as they are presented in the Study Report (optional). If a protein amount and volume used are provided, calculate the concentration by dividing the amount by the volume (*e.g.*, 0.1 mg/0.5 mL = 0.2 mg/mL).

Comment [RDB5]: Is this conversion required?

Protein concentration

0.2 mg/mL

5.3 **Test system preparation:** Select one of the following from the drop-down menu (select one; optional):

- **In-house preparation** – select this when the *in vitro* test system used was prepared in house
- **Commercially available** – select this when the *in vitro* test system used originally provided by a commercial vendor

5.4 **Test system lot number**: If provided, enter the test system lot number for those that were provided by a commercial vendor (optional).

Test system lot number

06103045

5.5 **Incubation volume**: Enter the total volume used in the incubation, specify the units as they are presented in the Study Report (optional). If volumes were listed in steps, the total incubation volume may be calculated by adding the volumes used in each step (*e.g.*, 100 µL buffer + 10 µL NADPH + 40 µL compound tested + 50 µL precipitant used = 200 µL total volume).

Incubation volume

200 µL

5.6 **Incubation time**: Enter the duration of the incubation, specify the units as they are presented in the Study Report (optional). This duration implies the presence of all necessary components of the incubation (*i.e.*, the enzyme, the object, the precipitant, and if used, co-factors). Specify pH for experiments using conditions other than pH 7.4

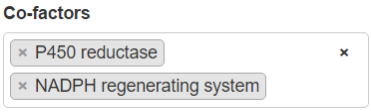
Incubation time

5 min

6 Incubation time

30 min at pH 6.8

5.7 **Co-factors**: Select co-factors used in the incubation from the drop-down list provided. Multiple co-factors may be selected as needed (select many; optional).



5.8 **Co-substrates**: Select co-substrates used to study enzyme activity from the drop-down list provided (select many; optional).

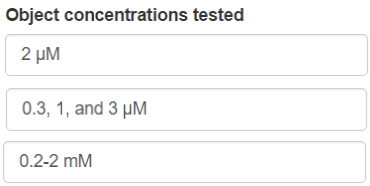
5.9 **Protein linearity**: Select one of the following from the drop-down menu (select one; optional):

- **Available** – select this when the linearity of product formation or substrate depletion with protein concentration is tested
- **Not available** - select this when no indication of testing linearity of product formation or substrate depletion with protein concentration is provided

5.10 **Time linearity**: Select one of the following from the drop-down menu (select one; optional):

- **Available** – select this when the linearity of product formation or substrate depletion with incubation time is tested
- **Not available** - select this when no indication of testing linearity of product formation or substrate depletion with incubation time is provided

5.11 **Object concentrations tested**: Enter the object concentration(s) used in the incubation, specify the units as they are presented in the Study Report (optional). Enter only the study vehicle control (i.e. not the positive or negative control) as the object. Enter the details regarding the positive/negative control in the Additional Information section under this tab. A single concentration, multiple concentrations or a range of concentrations may be entered, see below for examples. If possible, avoid entering "0" as a starting concentration, but rather, use the lowest concentration provided as the starting concentration (*i.e.*, do not enter 0-2 mM, but rather enter 0.2-2 mM).



5.12 **Precipitant concentrations tested:** Enter the precipitant concentration(s) used in the incubation, specify the units as they are presented in the Study Report (optional). A single concentration, multiple concentrations or a range of concentrations may be entered.

Precipitant concentrations tested

5 nM

2, 10, and 50 µM

1-10 µM

****

The following fields are to be used for mechanism-based or time-dependent inhibition studies only:

5.13 Precipitant pre-incubation volume (optional): Enter the total volume used for the primary incubation (inactivation of the enzyme), specify the units as they are presented in the Study Report (*e.g.*, 100 µL).

5.14 Precipitant pre-incubation time (optional)**:** Enter the duration used for the primary incubation (inactivation of the enzyme), specify the units as they are presented in the Study Report (*e.g.*, 10 min).

5.15 Precipitant pre-incubation condition (select one; optional)**:**

- **NADPH with precipitant** – select this when both NADPH and the precipitant are present in the primary incubation (inactivation of the enzyme)
- **NADPH with no precipitant** – select this when NADPH but not the precipitant is present in the primary incubation (inactivation of the enzyme)
- **No NADPH with precipitant** – select this when the precipitant but not NADPH is present in the primary incubation (inactivation of the enzyme)
- **No NADPH with no precipitant** – select this when neither NADPH nor the precipitant is present in the primary incubation (inactivation of the enzyme)

5.16 Secondary enzyme activity incubation volume (optional)**:** Enter the total volume used for the secondary incubation (measurement of enzyme activity), specify the units as they are presented in the Study Report (*e.g.*, 200 µL).

5.17 Secondary enzyme activity incubation time (optional)**:** Enter the duration used for the secondary incubation (measurement of enzyme activity), specify the units as they are presented in the Study Report (*e.g.*, 30 min).

5.18 Dilution factor (optional)**:** Enter the dilution factor used going from the primary to the secondary incubation (*e.g.*, 1:10).

****

5.19 Additional information (optional)**:** As needed, add any other information that is important to the experimental conditions, but that were not detailed in the fields above. If reporting a vehicle control, enter the details regarding the positive/negative control in this section. In the public view, this section will appear before any of the other experimental details entered.

Examples of additional information might include issues limiting the experimental design (*e.g.*, solubility), deviations from physiological pH (*e.g.*, studies were conducted at pH 6.0), details regarding substrate cocktail assays, etc.

Additional information

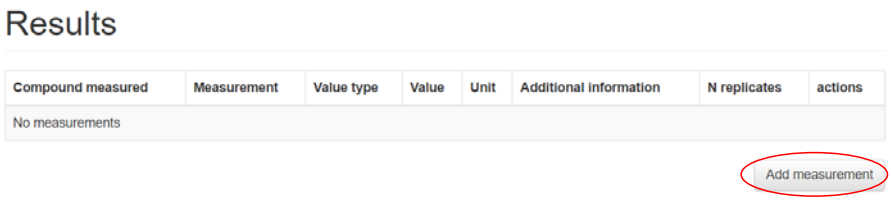
File Edit Insert View Format Table Tools

Formats

Due to solubility issues, the highest tested concentration of green tea leaf was 218 µg/mL.

6 RESULTS

6.1 Use the **Add measurement** function to add a new measurement to the table of results.



The object compound (or metabolite) name selected in the experiment page will automatically be populated in the **Compound measured** field.

6.2 Select a **Measurement type** (select one; required) from the drop-down list, the associated **Unit** (select one; required) and the **Value Type** (select one; required) based on the available data in the Study Report. Use separate entries for each type of measurement. Available measurement types include:

Measurement type	Selection criteria
% Inhibition$_{pre\text{-}incubation}$	The percent inhibition is reported during the pre-incubation phase of a mechanism-based or time-dependent inhibition assay.
% Inhibition$_{co\text{-}incubation}$	The percent inhibition is reported during the co-incubation phase of a mechanism-based or time-dependent inhibition assay.
% Inhibition	Percent inhibition is reported.
Ki total	Ki corresponding to the total (bound and unbound) precipitant is reported. For published literature: If apparent Ki is reported without information regarding protein binding, select Ki total and make a note in the additional information section.
Ki unbound	Ki corresponding to the unbound precipitant is reported.
$IC_{50\ pre\text{-}incubation}$	The IC_{50} value reported during the pre-incubation phase of a mechanism-based or time-dependent inhibition assay.
$IC_{50\ co\text{-}incubation}$	The IC_{50} value reported during the co-incubation phase of a mechanism-based or time-dependent inhibition assay.
IC_{50}	IC_{50} value is reported.
IC_{50} fold-shift	The IC_{50} fold-shift (fold-change) is reported.
K_{inact}	For mechanism-based or time-dependent inhibition, the K_{inact} is reported.

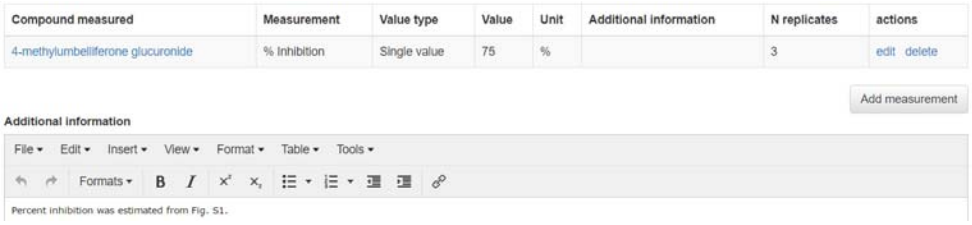
K_I	For mechanism-based or time-dependent inhibition, the K_I is reported.
K_{inact}/K_I	For mechanism-based or time-dependent inhibition, the K_{inact}/K_I is reported or this value can be calculated from the K_{inact} and K_I values provided.

According to the selections, appropriate fields will appear, including the following:

6.2.1 **Value** (select one; required) – based on the Study Report choose mean, median, or single value (mean or median is not specified) for the parameter to be entered. Before the value field, select ">", "≥", "<", or "≤" when provided in the Study Report; "=" is the default if no selection is made.

Comment [JS6]: Chris has not yet implemented this

For data from published articles: If the **percent inhibition** value is not explicitly stated in the article it can often be estimated from presented figures. Estimate the percent inhibition and in the additional information box located directly below the results, state that the value entered was estimated and specify the information source.



6.2.2 **Variability** (required) – enter the standard error of the mean (**SEM**), percent coefficient of variation (**%CV**), standard deviation (**SD**), 90% or 95% confidence interval (**90% CI**, **95% CI**) or **range** associated with the value.

6.2.3 Enter the total number of **(N) replicates** (required) used in the study (e.g., enter 1 when only one test was conducted, 3 when a total of 3 replicates were used, etc.).

Comment [JS7]: Ask chris to add a range as an input option for N replicates and to make this field optional as this is not always provided in published literature

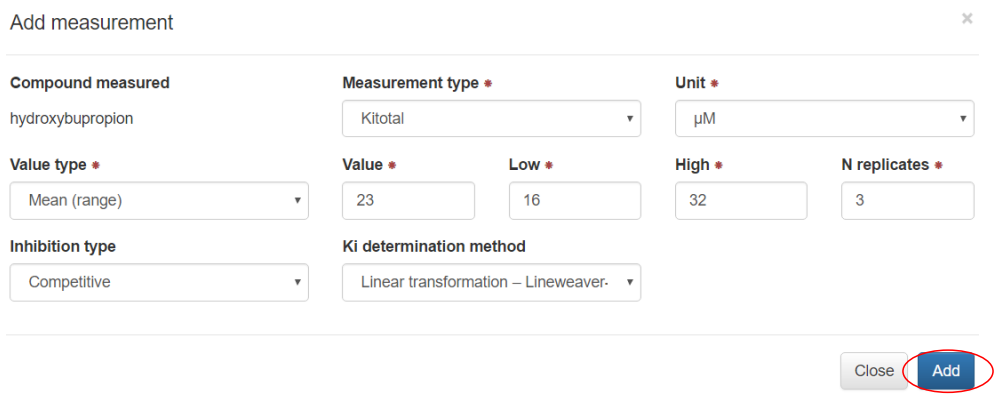
6.2.4 When statistical tests are conducted, select a significance level of the **P value** tested or **not significant** (optional) when the null hypothesis is true. If the authors give a P value that is not available in the drop-down menu, chose the level of significance that is true (e.g., if P = 0.0009 in the Study report, choose P < 0.001).

6.2.5 **Ki determination**: according to the Study Report, select the method used to determine Ki from the following options:

- Nonlinear least-squares regression
- Linear transformation – Eadie-Hofstee plot

- Linear transformation – Lineweaver-Burk plot
- Linear transformation – Dixon plot
- Graphic Read
- Not Available

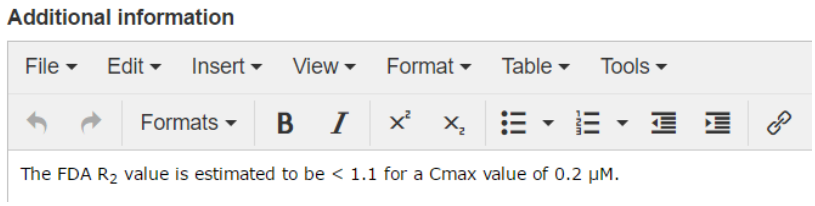
6.3 When all PK measurements have been entered for that entry, click **Add**.

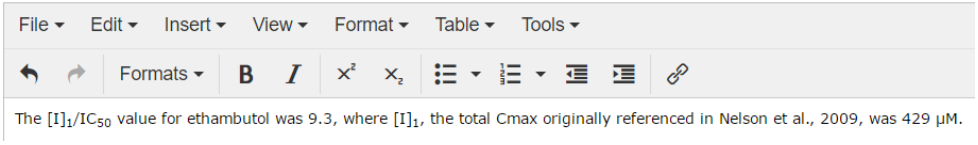


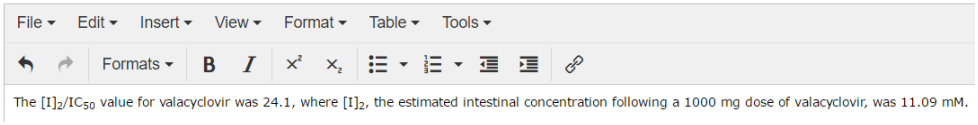
6.4 **Additional Information:** as needed, add any other information that is important to the result, but that were not detailed in the results table. If reporting a vehicle control, enter the details regarding the positive/negative control in this section.

For example,

In vivo DDI predictions ($[I]/IC_{50}$ or $[I]/K_i$ ratios, R_2 values, etc.) provided in the Study Report. Indicate the C_{max} and dosing information provided, otherwise, cite the original references (First Author, Year).

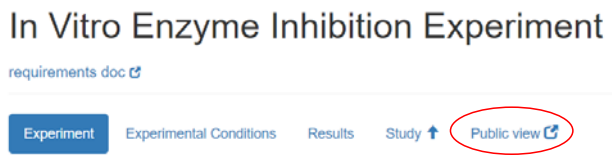






Click Submit to save the entries.

After submitting the study entry, it can be viewed as it will appear to the public by clicking on the "Public View" function near the top of the page.



Note regarding units: For consistency use the following abbreviations for the specified units below. If a unit is not listed below, use the units specified in the Study Report.

Unit	Abbreviation
hour(s)	h
minute(s)	min
second(s)	s
day(s)	day(s)
liter	L
per unit	/unit (*e.g.*, /min)
micro	µ
fold	-fold (*e.g.*, 3.2-fold)
exponents	^ (*e.g.*, 10^-6)
less than, less than or equal to	< , ≤
greater than, greater than or equal to	> , ≥
plus or minus	±

- Use molar concentration rather than moles per liter (i.e., use µM rather than µmol/L). In the case of natural products, the use if grams per liter (i.e., µg/mL) may be necessary.
- Do not convert gram concentrations (*e.g.*, µg/mL) to molar concentrations (*e.g.*, µM), even if the molecular weight of the compound is provided.
- If the units provided for a given field are different from the units in its corresponding drop-down menu, convert the units provided in the study report to the units provided in the drop-down menu. If this is not possible (for example, µg/mL cannot be converted to µM for natural product

Comment [RDB8]: Please clarify. Does this mean don't use molar units per L? Are there any conversions that the computer can do to make it simpler for the annotator and likely more accurate and consistent overall?

mixtures because there is not a molecular weight available for the conversion), add the new unit to the drop-down menu.

Table S1. Data elements and measurement types represented in the NaPDI Center repository. Data elements are preser chemical characterization of the material (Cha), metabolomics (Met), in vitro enzyme induction (Ind), inhibition (Inh), kir inhibition (Inh), iinetics (kin), clinical interaction and pharmacokinetics. Data elements are proposed to be filled "x", are depending on experiments type.

	Data elements	Chemistry		*In vitro*				
		Cha	Met	Enzyme				Trar
				Ind	Inh	Kin	Scr	Ind
STUDY	Natural product name	x	x	x	x	x	x	x
	Unique identifier	x	x	x	x	x	x	x
	Subject of study (natural product, constituent)	x	x	x	x	x	x	x
	Study name (Title)	x	x	x	x	x	x	x
	NaPDI study identification	x	x	x	x	x	x	x
	Study source type (published report, manuscript *in prep* or *submit* , unpublished data submitted through a NaPDI form)	x	x	x	x	x	x	x
	Pubmed ID	x	x	x	x	x	x	x
	Embase accession number	x	x	x	x	x	x	x
	Overall summary	x	x	x	x	x	x	x
	Link to pharmacology studies: Lab product code	x	x	-	-	-	-	-
	Link to pharmacology studies: Manufacturer (will be encoded)	x	x	-	-	-	-	-
	Link to pharmacology studies: Lot number	x	x	-	-	-	-	-
	Link to pharmacology studies: Product form	x	x	-	-	-	-	-
	Link to pharmacology studies: Product name (will be encoded)	x	x	-	-	-	-	-
	Link to pharmacology studies: Size	x	x	-	-	-	-	-
	Internal: Research Organization information	x	x	x	x	x	x	x
	Internal: Research Organization study ID	x	x	x	x	x	x	x
	Internal: Dates study conducted	x	x	x	x	x	x	x
	Internal: Additional comments	x	x	x	x	x	x	x
	Revision history	x	x	x	x	x	x	x
	Status (Draft, Pending review, Published)	x	x	x	x	x	x	x
EXPERIMENT	Unique identifier	x	x	x	x	x	x	x
	Experiment name (Title)	x	x	x	x	x	x	x
	Overall effect (i.e., non induction/ induction/down regulation)	-	-	x	x	x	x	x
	Control data (yes or no)	-	-	x	x	x	x	x
	IC50 shift data (yes or no)	-	-	-	x	-	-	-
	Research organization's overall effect cutoff	-	-	x	x	x	-	-
	Research organization's experiment ID	x	x	x	x	x	x	x
	Additional information	x	x	x	x	x	x	x
	Experimental conditions comment	x	x	x	x	x	x	x
	Experimental results comment	x	x	x	x	x	x	x
	Internal: Additional comments	x	x	x	x	x	x	x
	Object drug	-	-	x	x	x	x	x
	Object metabolite measured	-	-	x	x	x	x	-

	Precipitant (NP)	-	-	x	x	-	-	x
	Cytochrome B5	-	-	-	-	x	-	-
	Study of experiment	x	x	x	x	x	x	x
	Experiment type (in vitro, in vivo, characterization of material, metabolomics, etc.)	x	x	x	x	x	x	x
	Test system (pooled human liver microsomes, recombinant enzymes, hepatocytes, etc.)	-	-	x	x	x	x	x
	Related IC50 shift experiment	-	-	-	x	-	-	-
	Related control data experiment	-	-	x	x	x	x	x
	Natural product sample	x	-	-	-	-	-	-
	Lot number	x	x	x	x	x	x	-
	Lab product code	x	x	-	-	-	-	-
	Product form	x	x	-	-	-	-	-
	Material preparation (mass of sample, volume of extraction vessel, solvent, volume of solvent, temperature of storage)	x	x	-	-	-	-	-
	Material preparation additional information	x	x	-	-	-	-	-
	NMR analysis (instrument, nucleus, field strength, solvent, sample concentration)	x	x	-	-	-	-	-
	Manufacturer/source	-	-	-	-	-	-	-
	Natural product characterization	-	-	-	-	-	-	-
	Year sourcing was completed	-	-	-	-	-	-	-
	Natural product additional information	-	-	-	-	-	-	-
	Mass Spectrometry analysis (instrument, sample concentration, ionization, ionization mode, LC instrument, solvent system, gradient, flow rate, column)	x	x	-	-	-	-	-
	Mass spectrometry additional information	x	x	-	-	-	-	-
	Metabolite quantification (method, solvent, number of calibration points, sample concentration range, curve fitting method, weighting method)	x	x	-	-	-	-	-
	Induction measurement level (mRNA expression, protein expression, enzyme activity, transporter activity)	-	-	x	-	-	-	x
	Cell density	-	-	x	x	x	x	x
	Plate type	-	-	-	-	-	-	-
	Days after plating	-	-	-	-	-	-	-
	Passage number	-	-	-	-	-	-	-
	Viability test (yes or no)	-	-	x	-	-	-	x
	Protein concentration	-	-	-	x	x	x	-
	Number of livers	-	-	x	-	-	-	-
	Test system preparation (in house or commercial)	-	-	-	x	x	x	-
	NP concentrations tested	-	-	x	x	-	-	x
	Incubation volume	-	-	-	x	x	x	-
	Incubation time	-	-	x	x	x	x	x
	Incubation temperature	-	-	-	-	-	-	-
	Incubation pH	-	-	-	-	-	-	-
	Method for determination	-	-	x	-	x	x	x
	Protein linearity	-	-	-	x	x	x	-
	Co-factors	-	-	-	x	x	x	-
	Co-susbstrate	-	-	-	x	x	x	-
	Time linearity	-	-	-	x	x	x	-
RIMENT CONDITIONS	Object drug concentration tested	-	-	-	x	x	x	-

EXPEF	NP pre-incubation volume	-	-	-	x	-	-	-
	NP pre-incubation time	-	-	-	x	-	-	-
	NP pre-incubation condition (with NADPH or not)	-	-	-	x	-	-	-
	Secondary enzyme activity incubation volume	-	-	-	x	-	-	-
	Secondary enzyme activity incubation time	-	-	-	x	-	-	-
	Dilution factor	-	-	-	x	-	-	-
	Study design (parallel, double-blind, ect…)	-	-	-	-	-	-	-
	Demographic characteristics	-	-	-	-	-	-	-
	Lifestyle factors	-	-	-	-	-	-	-
	Ethnicity	-	-	-	-	-	-	-
	Phenotype	-	-	-	-	-	-	-
	Genotype	-	-	-	-	-	-	-
	Number of subjects	-	-	-	-	-	-	-
	Population additional information	-	-	-	-	-	-	-
	Object pharmacokinetics samples quality concerns	-	-	-	-	-	-	-
	Times of Pharmacokinetics samples for object	-	-	-	-	-	-	-
	Natural product pharmacokinetics samples quality concerns	-	-	-	-	-	-	-
	Times of Pharmacokinetics samples for natural product	-	-	-	-	-	-	-
	Administration route object drug	-	-	-	-	-	-	-
	Administration route NP	-	-	-	-	-	-	-
	Formulation object drug	-	-	-	-	-	-	-
	Formulation NP	-	-	-	-	-	-	-
	Total daily dose object drug	-	-	-	-	-	-	-
	Total daily dose NP	-	-	-	-	-	-	-
	Prandial state	-	-	-	-	-	-	-
	Prandial state comment	-	-	-	-	-	-	-
	Interval/frequency object drug	-	-	-	-	-	-	-
	Interval/frequency NP	-	-	-	-	-	-	-
	Duration object drug	-	-	-	-	-	-	-
	Duration NP	-	-	-	-	-	-	-
	Pharmacodynamic protocol	-	-	-	-	-	-	-
	Pharmacodynamic measurement classes	-	-	-	-	-	-	-
	Additional information	x	x	x	x	x	x	x
RESULTS	Compounds measured	x	x	x	x	x	x	x
	Measurement type (quantity, EC50, % inhibition, ect..) - *See above for the complete list*	x	x	x	x	x	x	x
	Unit (%, mg/g sample, fold,)	x	x	x	x	x	x	x
	Value type (single value, mean or median with range, SD, CV%, 90% and 95% CI)	x	x	x	x	x	x	x
	Value comparator (=, <, >, ≤, ≥)	x	x	x	x	x	x	x
	PCA methods (missing value, filtering, normalization, transformation, scaling)	-	x	-	-	-	-	-
	PCA plot: analysis type	-	x	-	-	-	-	-
	PCA plot: principal components	-	x	-	-	-	-	-
	PCA plot: number of dimensions (2D, 3D)	-	x	-	-	-	-	-
	Value	x	x	x	x	x	x	x
	Variability	-	-	x	x	x	x	x
	Number of replicates	-	-	x	x	x	x	x

p-value	-	-	x	x	x	x	x
Images (file name, image title, description, additonal information)	x	x	-	-	-	-	-
Pharmacodynamic results	-	-	-	-	-	-	-
Adverse event classes	-	-	-	-	-	-	-
Safety results	-	-	-	-	-	-	-
Additionnal information	x	x	x	x	x	x	x

terization to Clinical Studies",

ıted for all experiment type of the NaPDI Center repository, for
ıetics (kin), screen (Scr), in vitro transporter induction (Ind),
required to be filled " x" or are not available to be filled "-"

		In vivo			
ısporter		Int	Pha		Measurement Types
Inh	Kin				
x	x	x	x		K_m
x	x	x	x		V_{max}
x	x	x	x		$CL_{int\ total}$
x	x	x	x		$CL_{int\ unbound}$
x	x	x	x		Percent bound
x	x	x	x		Metabolic rate
x	x	x	x		% parent remaining
x	x	x	x		EC_{50}
x	x	x	x		E_{max}
-	-	-	-		Change from vehicle control
-	-	-	-		Change from positive control
-	-	-	-		% Inhibition
-	-	-	-		IC_{50}
-	-	-	-		Ki_{total}
-	-	-	-		$Ki_{unbound}$
x	x	x	x		% Inhibition $_{pre\text{-}incubation}$
x	x	x	x		% Inhibition $_{co\text{-}incubation}$
x	x	x	x		$IC_{50\ pre\text{-}incubation}$
x	x	x	x		$IC_{50\ co\text{-}incubation}$
x	x	x	x		IC_{50} -fold shift
x	x	x	x		K_{inact}
x	x	x	x		K_I
x	x	x	x		K_{inact} / K_I
X	X	X	-		Change in efflux compared with vehicle control
x	x	-	-		Change in efflux compared with positive control
-	-	-	-		Change in accumulation compared with vehicle control
x	x	-	-		Change in accumulation compared with positive control
x	x	x	x		P_{app} A-B Vector Control
x	x	x	x		P_{app} A-B Transfected
x	x	x	x		P_{app} A-B Caco-2
x	x	x	x		P_{app} B-A Vector Control
x	x	x	x		P_{app} B-A Transfected
X	X	x	-		P_{app} B-A Caco-2
-	-	-	-		Ratio P_{app}B-A / P_{app}A-B Vector Control

x	x	x	-	Ratio P_{app}B-A / P_{app}A-B Transfected
-	-	-	-	Ratio P_{app}B-A / P_{app}A-B Caco-2
x	x	x	x	Ratio Transfected / Vector Control
x	x	x	x	Permeability Rate
X	X	-	-	Efflux Ratio
-	-	-	-	Fold Accumulation Vector Control
x	x	-	-	Fold Accumulation Transfected
-	-	-	-	Ratio of Fold Accumulation Transfected / Vector Control
-	-	x	x	Accumulation Rate
-	-	-	-	$K_{m\ total}$
-	-	-	-	$K_{m\ unbound}$
-	-	-	-	V_{max} or J_{max}
-	-	-	-	V_{max} / K_m or J_{max} / K_m
-	-	-	-	Fit Model
-	-	x	x	Hill Coefficient
-	-	x	x	Accumulation
-	-	x	x	AUC_{Tau}
-	-	x	x	$AUC_{(0\text{-}infinity)}$
-	-	-	-	$AUC_{(0\text{-}tn)}$
-	-	-	-	$AUC_{(0\text{-}t)}$
-	-	-	-	AUC ratio (metabolite/parent)
-	-	-	-	AUC ratio (parent/metabolite)
x	x	-	-	C (plasma)
x	x	-	-	C ratio (metabolite/parent)
x	x	-	-	C ratio (parent/metabolite)
x	x	-	-	CL (renal)
x	x	-	-	CL/F
x	x	-	-	C_{max}
-	-	-	-	$C_{ss\ avg}$
-	-	-	-	$C_{ss\ trough}$
x	-	-	-	Fraction bound in plasma
-	-	-	-	Fraction unbound in plasma
x	x	-	-	Half-life (terminal)
x	x	-	-	MRT
x	x	-	-	T_{max}
-	-	-	-	Cumulative Urinary Excretion (% Dose)
-	-	-	-	Urinary molar ratio (metabolite/parent)
-	-	-	-	Urinary molar ratio (parent/metabolite)
-	-	-	-	V_d/F
-	-	-	-	AUC ratio (treatment/control)
x	x	-	-	AUC ratio (control/treatment)

-	-	-	-	C_{max} ratio (treatment/control)
-	-	-	-	C_{max} ratio (control/treatment)
-	-	-	-	Half-life ratio (treatment/control)
-	-	-	-	Half-life ratio (control/treatment)
-	-	-	-	AUC (dose normalized)
-	-	-	-	Percentage of control activity
-	-	x	x	α
-	-	x	x	Quantity
-	-	x	x	
-	-	x	x	
-	-	x	x	
-	-	x	x	
-	-	x	x	
-	-	x	x	
-	-	x	x	
-	-	x	x	
-	-	x	-	
-	-	x	-	
-	-	x	-	
-	-	x	x	
-	-	x	-	
-	-	x	x	
-	-	x	-	
-	-	x	x	
-	-	-	x	
-	-	-	x	
-	-	x	-	
-	-	x	x	
-	-	x	-	
-	-	x	x	
-	-	x	x	
-	-	x	x	
x	x	x	x	
x	x	x	x	
x	x	x	x	
x	x	x	x	
x	x	x	x	
x	x	x	x	
-	-	-	-	
-	-	-	-	
-	-	-	-	
-	-	-	-	
x	x	x	x	
x	x	x	x	
x	x	x	x	

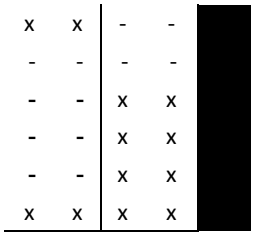


Table S2. Data in the NaPDI Center repository on Cannabis sativa as of

Study unique identifier	Unique identifier	Natural product binomial
NPDI-0mD33A	NPDI-Hko3aA	Cannabis sativa
NPDI-1wiJBw	NPDI-29ER6A	Cannabis sativa
NPDI-1wiJBw	NPDI-2LIXDQ	Cannabis sativa
NPDI-1wiJBw	NPDI-Aasqdw	Cannabis sativa
NPDI-1wiJBw	NPDI-cqaAMA	Cannabis sativa
NPDI-1wiJBw	NPDI-DZj9Zg	Cannabis sativa
NPDI-1wiJBw	NPDI-E7xthw	Cannabis sativa
NPDI-1wiJBw	NPDI-loxesQ	Cannabis sativa
NPDI-1wiJBw	NPDI-lx-KKg	Cannabis sativa
NPDI-1wiJBw	NPDI-jHdxpA	Cannabis sativa
NPDI-1wiJBw	NPDI-mbNW9A	Cannabis sativa
NPDI-1wiJBw	NPDI-mLsAbQ	Cannabis sativa
NPDI-1wiJBw	NPDI-olqNRw	Cannabis sativa
NPDI-1wiJBw	NPDI-oZGcUg	Cannabis sativa
NPDI-1wiJBw	NPDI-PaO28A	Cannabis sativa
NPDI-1wiJBw	NPDI-spUvqw	Cannabis sativa
NPDI-2P3dUg	NPDI-tRoTQw	Cannabis sativa
NPDI-8lgFiA	NPDI-a65Zxg	Cannabis sativa
NPDI-8lgFiA	NPDI-PwGUoQ	Cannabis sativa
NPDI-8lgFiA	NPDI-ypo3GA	Cannabis sativa
NPDI-9V_SXw	NPDI-9kN5_g	Cannabis sativa
NPDI-9V_SXw	NPDI-fw_WMw	Cannabis sativa
NPDI-9V_SXw	NPDI-GEE68Q	Cannabis sativa
NPDI-9V_SXw	NPDI-Z_m2jA	Cannabis sativa
NPDI-ahQtSQ	NPDI-7RWWrg	Cannabis sativa
NPDI-ahQtSQ	NPDI-JnMHww	Cannabis sativa
NPDI-ahQtSQ	NPDI-lNsNoQ	Cannabis sativa
NPDI-ahQtSQ	NPDI-PWUeog	Cannabis sativa
NPDI-ahQtSQ	NPDI-qeGJYg	Cannabis sativa
NPDI-ahQtSQ	NPDI-uUyadQ	Cannabis sativa
NPDI-Asg_wA	NPDI-xU8LWA	Cannabis sativa
NPDI-BvR0Pw	NPDI-6v65qQ	Cannabis sativa
NPDI-BvR0Pw	NPDI-R1QKZg	Cannabis sativa
NPDI-CAApFQ	NPDI-_k7VAQ	Cannabis sativa
NPDI-CAApFQ	NPDI-3Crf-w	Cannabis sativa
NPDI-CAApFQ	NPDI-3EHgSg	Cannabis sativa
NPDI-CAApFQ	NPDI-8HM-ew	Cannabis sativa
NPDI-CAApFQ	NPDI-A4_kwg	Cannabis sativa
NPDI-CAApFQ	NPDI-E2Dy1A	Cannabis sativa
NPDI-CAApFQ	NPDI-egkFFQ	Cannabis sativa
NPDI-CAApFQ	NPDI-es-pWA	Cannabis sativa

NPDI-CAApFQ	NPDI-F14zbg	Cannabis sativa
NPDI-CAApFQ	NPDI-F2AXtQ	Cannabis sativa
NPDI-CAApFQ	NPDI-FGSLRQ	Cannabis sativa
NPDI-CAApFQ	NPDI-ILAq5w	Cannabis sativa
NPDI-CAApFQ	NPDI-k7I3rg	Cannabis sativa
NPDI-CAApFQ	NPDI-L4dcwg	Cannabis sativa
NPDI-CAApFQ	NPDI-PMEwbg	Cannabis sativa
NPDI-CAApFQ	NPDI-QtzrqQ	Cannabis sativa
NPDI-CAApFQ	NPDI-w7jBLw	Cannabis sativa
NPDI-CAApFQ	NPDI-wcUiKQ	Cannabis sativa
NPDI-cM9pfg	NPDI-8Ej-Bg	Cannabis sativa
NPDI-cM9pfg	NPDI-EqzxjQ	Cannabis sativa
NPDI-cM9pfg	NPDI-G8_czw	Cannabis sativa
NPDI-cM9pfg	NPDI-gOdMHw	Cannabis sativa
NPDI-cM9pfg	NPDI-NC4pjQ	Cannabis sativa
NPDI-cM9pfg	NPDI-UlHjqQ	Cannabis sativa
NPDI-d4aGfw	NPDI--0E9EQ	Cannabis sativa
NPDI-d4aGfw	NPDI-2KocMg	Cannabis sativa
NPDI-d4aGfw	NPDI-8d0Lug	Cannabis sativa
NPDI-d4aGfw	NPDI-a3nUTg	Cannabis sativa
NPDI-d4aGfw	NPDI-AIeEmg	Cannabis sativa
NPDI-d4aGfw	NPDI-gAcr3g	Cannabis sativa
NPDI-d4aGfw	NPDI-LI0O-A	Cannabis sativa
NPDI-d4aGfw	NPDI-sciDeA	Cannabis sativa
NPDI-d4aGfw	NPDI-t5Bygg	Cannabis sativa
NPDI-DlD-bA	NPDI-hQQnWg	Cannabis sativa
NPDI-DlD-bA	NPDI--NblVQ	Cannabis sativa
NPDI-eJTztA	NPDI-1B-DfQ	Cannabis sativa
NPDI-eJTztA	NPDI-CtgCHg	Cannabis sativa
NPDI-eJTztA	NPDI-GqHdbQ	Cannabis sativa
NPDI-eJTztA	NPDI-IW6BRg	Cannabis sativa
NPDI-eJTztA	NPDI-RY8JgQ	Cannabis sativa
NPDI-eJTztA	NPDI-S43ljQ	Cannabis sativa
NPDI-eJTztA	NPDI-uPtFxA	Cannabis sativa
NPDI-eJTztA	NPDI-VNa1xQ	Cannabis sativa
NPDI-EngCtg	NPDI-4ZUTtw	Cannabis sativa
NPDI-EngCtg	NPDI-yqEgVA	Cannabis sativa
NPDI-euNEwQ	NPDI-3VIAiw	Cannabis sativa
NPDI-euNEwQ	NPDI-4htiMA	Cannabis sativa
NPDI-euNEwQ	NPDI-GRyerw	Cannabis sativa
NPDI-FhBdoQ	NPDI-LCPweA	Cannabis sativa
NPDI-FhBdoQ	NPDI-S4_OQA	Cannabis sativa
NPDI-gTt8Dw	NPDI-UlPhZQ	Cannabis sativa
NPDI-i4m0FA	NPDI-soqMrQ	Cannabis sativa
NPDI-ieYYdA	NPDI-0g58zw	Cannabis sativa
NPDI-ieYYdA	NPDI-8jlF2g	Cannabis sativa
NPDI-ieYYdA	NPDI-b-kubA	Cannabis sativa

NPDI-ieYYdA	NPDI-ckGWRw	Cannabis sativa
NPDI-ieYYdA	NPDI-F3DjaQ	Cannabis sativa
NPDI-ieYYdA	NPDI-Hsp-vg	Cannabis sativa
NPDI-ieYYdA	NPDI-iDzluw	Cannabis sativa
NPDI-ieYYdA	NPDI-KQoVKg	Cannabis sativa
NPDI-ieYYdA	NPDI-p2jqFw	Cannabis sativa
NPDI-ieYYdA	NPDI-THQe_g	Cannabis sativa
NPDI-ieYYdA	NPDI-XBXjow	Cannabis sativa
NPDI-ieYYdA	NPDI-y29wsw	Cannabis sativa
NPDI-iHWMgQ	NPDI-8vislA	Cannabis sativa
NPDI-iHWMgQ	NPDI-ens_Gw	Cannabis sativa
NPDI-iHWMgQ	NPDI-FmAizA	Cannabis sativa
NPDI-iHWMgQ	NPDI-PS8_LQ	Cannabis sativa
NPDI-iHWMgQ	NPDI-yszOMw	Cannabis sativa
NPDI-iHWMgQ	NPDI-zkYApA	Cannabis sativa
NPDI-l0yevQ	NPDI-Q2pa5g	Cannabis sativa
NPDI-l0yevQ	NPDI-zu7hCg	Cannabis sativa
NPDI-lY9NZQ	NPDI-4qS0VQ	Cannabis sativa
NPDI-lY9NZQ	NPDI-jW07Iw	Cannabis sativa
NPDI-lY9NZQ	NPDI-qHswZw	Cannabis sativa
NPDI-m-U3YQ	NPDI-3LZeDA	Cannabis sativa
NPDI-m-U3YQ	NPDI-dsHL7w	Cannabis sativa
NPDI-m-U3YQ	NPDI-ZFfQJg	Cannabis sativa
NPDI-muoDdQ	NPDI-uz4EAA	Cannabis sativa
NPDI-qOTUkQ	NPDI-J5A-Vg	Cannabis sativa
NPDI-qOTUkQ	NPDI-qhVkgQ	Cannabis sativa
NPDI-Rvn9SQ	NPDI-42-g8Q	Cannabis sativa
NPDI-Rvn9SQ	NPDI-5Fz7kg	Cannabis sativa
NPDI-Rvn9SQ	NPDI-8flCOQ	Cannabis sativa
NPDI-Rvn9SQ	NPDI-abEayg	Cannabis sativa
NPDI-Rvn9SQ	NPDI-EYnQkA	Cannabis sativa
NPDI-Rvn9SQ	NPDI-I4dv_g	Cannabis sativa
NPDI-Rvn9SQ	NPDI-IQtjvw	Cannabis sativa
NPDI-Rvn9SQ	NPDI-M13k5Q	Cannabis sativa
NPDI-Rvn9SQ	NPDI-M8-Oxw	Cannabis sativa
NPDI-Rvn9SQ	NPDI-qmmKqA	Cannabis sativa
NPDI-Rvn9SQ	NPDI-rbqhsA	Cannabis sativa
NPDI-Rvn9SQ	NPDI-RCBEtw	Cannabis sativa
NPDI-Rvn9SQ	NPDI-THVK4A	Cannabis sativa
NPDI-Rvn9SQ	NPDI-uxfWFg	Cannabis sativa
NPDI-Rvn9SQ	NPDI-v8ghug	Cannabis sativa
NPDI-Rvn9SQ	NPDI-VpD-Xg	Cannabis sativa
NPDI-Rvn9SQ	NPDI-YQ1c2Q	Cannabis sativa
NPDI-Rvn9SQ	NPDI-Yr3jng	Cannabis sativa
NPDI-SiYA_A	NPDI-_jX3DQ	Cannabis sativa
NPDI-SiYA_A	NPDI-2TMzVA	Cannabis sativa
NPDI-SiYA_A	NPDI-4EVwQw	Cannabis sativa

NPDI-SiYA_A	NPDI-8_xKYg	Cannabis sativa
NPDI-SiYA_A	NPDI-9oyo4g	Cannabis sativa
NPDI-SiYA_A	NPDI-a9Sh7Q	Cannabis sativa
NPDI-SiYA_A	NPDI-AEDMtg	Cannabis sativa
NPDI-SiYA_A	NPDI-AWv-_A	Cannabis sativa
NPDI-SiYA_A	NPDI-d2rDLg	Cannabis sativa
NPDI-SiYA_A	NPDI-kJ7mIQ	Cannabis sativa
NPDI-SiYA_A	NPDI-wM7_CQ	Cannabis sativa
NPDI-SiYA_A	NPDI-Y9U8Tw	Cannabis sativa
NPDI-SiYA_A	NPDI-z3MwKw	Cannabis sativa
NPDI-SiYA_A	NPDI-ZM5Pkw	Cannabis sativa
NPDI-sUzV-g	NPDI-akOrWg	Cannabis sativa
NPDI-sUzV-g	NPDI-CWIhCg	Cannabis sativa
NPDI-sUzV-g	NPDI-GNkg_Q	Cannabis sativa
NPDI-sUzV-g	NPDI-GT0H0Q	Cannabis sativa
NPDI-sUzV-g	NPDI-PxRYvA	Cannabis sativa
NPDI-sUzV-g	NPDI-qk8qvw	Cannabis sativa
NPDI-sUzV-g	NPDI-Qoqt5Q	Cannabis sativa
NPDI-sUzV-g	NPDI-ToTRjw	Cannabis sativa
NPDI-TvFZMw	NPDI-6sB67w	Cannabis sativa
NPDI-TvFZMw	NPDI-PO4R-w	Cannabis sativa
NPDI-UaGLOg	NPDI-pvvgAw	Cannabis sativa
NPDI-Ujn_7A	NPDI-9ju4Lw	Cannabis sativa
NPDI-Ujn_7A	NPDI-BfJ7dA	Cannabis sativa
NPDI-Ujn_7A	NPDI-E6xHTA	Cannabis sativa
NPDI-Ujn_7A	NPDI-iJRQWg	Cannabis sativa
NPDI-Ujn_7A	NPDI-ZmjyHw	Cannabis sativa
NPDI-uPn_2w	NPDI-6t3-aw	Cannabis sativa
NPDI-uPn_2w	NPDI-P9f-Mw	Cannabis sativa
NPDI-uPn_2w	NPDI-RUuAkA	Cannabis sativa
NPDI-UXOaUA	NPDI-37uQKw	Cannabis sativa
NPDI-UXOaUA	NPDI-csAo1g	Cannabis sativa
NPDI-UXOaUA	NPDI-hnUjdg	Cannabis sativa
NPDI-UXOaUA	NPDI-I4ebig	Cannabis sativa
NPDI-UXOaUA	NPDI-px3AyQ	Cannabis sativa
NPDI-UXOaUA	NPDI-wx2mcg	Cannabis sativa
NPDI-vhBMSw	NPDI-7hkXUg	Cannabis sativa
NPDI-vhBMSw	NPDI-dh6TjQ	Cannabis sativa
NPDI-vhBMSw	NPDI-DpYeow	Cannabis sativa
NPDI-vhBMSw	NPDI-ILsKWw	Cannabis sativa
NPDI-vhBMSw	NPDI-JvqWDQ	Cannabis sativa
NPDI-vhBMSw	NPDI-jwN2Vw	Cannabis sativa
NPDI-vniY7Q	NPDI-59dZ4A	Cannabis sativa
NPDI-vniY7Q	NPDI-bM6NOQ	Cannabis sativa
NPDI-vniY7Q	NPDI-dvyC1w	Cannabis sativa
NPDI-vniY7Q	NPDI-Fqa3JA	Cannabis sativa
NPDI-vniY7Q	NPDI-Jb4JFA	Cannabis sativa

NPDI-vniY7Q	NPDI-jZO6oQ	Cannabis sativa
NPDI-vniY7Q	NPDI-KqafWg	Cannabis sativa
NPDI-vniY7Q	NPDI-LKS7Ow	Cannabis sativa
NPDI-vniY7Q	NPDI-mGu2ew	Cannabis sativa
NPDI-vniY7Q	NPDI-P2rdYg	Cannabis sativa
NPDI-vniY7Q	NPDI-V1SemA	Cannabis sativa
NPDI-vniY7Q	NPDI-vUechg	Cannabis sativa
NPDI-vniY7Q	NPDI-wt2yDg	Cannabis sativa
NPDI-vniY7Q	NPDI-XouN0Q	Cannabis sativa
NPDI-vniY7Q	NPDI-ZNPhvw	Cannabis sativa
NPDI-VYyv-A	NPDI-4tAywg	Cannabis sativa
NPDI-VYyv-A	NPDI-bxWjqg	Cannabis sativa
NPDI-VYyv-A	NPDI-DQGnJw	Cannabis sativa
NPDI-VYyv-A	NPDI-F-0XWg	Cannabis sativa
NPDI-VYyv-A	NPDI-FompNA	Cannabis sativa
NPDI-VYyv-A	NPDI-jYDUsw	Cannabis sativa
NPDI-VYyv-A	NPDI-RC8Kxw	Cannabis sativa
NPDI-VYyv-A	NPDI-v65nxg	Cannabis sativa
NPDI-VYyv-A	NPDI-XKoD2A	Cannabis sativa
NPDI-xYeUJQ	NPDI-noOe3w	Cannabis sativa
NPDI-xYeUJQ	NPDI-SCT2WA	Cannabis sativa
NPDI-xYeUJQ	NPDI-tUG7XA	Cannabis sativa
NPDI-Z6vbAA	NPDI-b6F8pQ	Cannabis sativa
NPDI-Z6vbAA	NPDI-DqfMEw	Cannabis sativa
NPDI-Z6vbAA	NPDI-pQrX0g	Cannabis sativa
NPDI-Z6vbAA	NPDI-wnmeug	Cannabis sativa
NPDI-zlH6uA	NPDI-jJ11Ig	Cannabis sativa
NPDI-zlH6uA	NPDI-otngFw	Cannabis sativa
NPDI-zlH6uA	NPDI-RPqAvQ	Cannabis sativa
NPDI-zlH6uA	NPDI-tjxX2A	Cannabis sativa
NPDI-ZqVOgw	NPDI-Rsay5Q	Cannabis sativa

ıral Product-Drug Interactions: from Chemical Characterization to Clinical Studies",

April 2020

Experiment title
Kinetic constants for 11-hydroxy-delta-9-THC formation
Down regulation of P-gp transporter (protein) by Cannabidiol
Down regulation of P-gp transporter (protein) by Cannabidiol
Induction of BCRP transporter (protein) by Cannabidiol
Inhibition of P-gp by Cannabidiol 10ÂµM
Down regulation of P-gp transporter (protein) by Cannabidiol
Down regulation of P-gp (mRNA) by Cannabidiol
Inhibition of P-gp by Cannabidiol 10 ÂµM
Induction of BCRP transporter (protein) by Cannabidiol
Induction (mRNA) of BCRP transporter with Cannabidiol
Induction of P-gp transporter (protein) by Cannabidiol
Inhibition of P-gp by Cannabidiol 25 ÂµM
Induction of BCRP transporter (protein) by Cannabidiol
Inhibition of P-gp by Cannabidiol 25 ÂµM
Non-induction of BCRP transporter (protein) by Cannabiodiol
Induction of BCRP transporter (mRNA) by Cannabidiol
Characterization of Cannabis extract (THC)
Mean THC Plasma Concentration with High Ethanol
Mean THC Concentration with Placebo
Mean THC Plasma Concentration with High Ethanol
Inhibition of CYP2C19 by Cannabidiol
Inhibition of CYP2C19 by Cannabidiol
Inhibition of CYP2C19 by Cannabidiol
Inhibition of CYP2C19 enzyme with Cannabidiol
Inhibition of ABCC1 by Cannabinol
Negligible inhibition of ABCC1 by Cannabinol
Negligible inhibition of ABCC1 by THC
Inhibition of ABCC1 by Cannabidiol
Negligible inhibition of ABCC1 by Cannabidiol
Negligible inhibition of ABCC1 by THC
THC PK
CBD
THC
THC-OMF
2H-CBD-omeprazole
CBDV-omeprazole
CBDD-(S)-mephenytoin
CBDD-OMF
2H-CBD-OMF
2H-CBD-(S)-Mephenytoin
CBD-(S)-Mephenytoin

THC-omeprazole
CBD-OMF
THC-(S)-Mephenytoin
CBD-omeprazole
CBDV-(S)-Mephenytoin
CBDD-omeprazole
CBDM-OMF
CBDM-omeprazole
CBDM-(S)-Mephenytoin
CBDV-OMF
CCRF-CEM: THC
CCRF-CEM: CBN
CEM/VLB100: CBN
CCRF-CEM: CBD
CEM/VLB100: THC
CEM/VLB100: CBD
Evaluation of Time-Dependent CES1 Inhibition by CBN (30 min)
Evaluation of Time-Dependent CES1 Inhibition by CBN (0 min)
Evaluation of Time-Dependent CES1 Inhibition by THC (30 min)
Inhibition of CES1 by CBD
Inhibition of CES1 by THC
Evaluation of Time-Dependent CES1 Inhibition by CBD (0 min)
Inhibition of CES1 by CBN
Evaluation of Time-Dependent CES1 Inhibition by CBD (30 min)
Evaluation of Time-Dependent CES1 Inhibition by THC (0 min)
Inhibited Hexobarbital metabolism with Cannabidiol (IV intake)
Inhibited Hexobarbital metabolism with Cannabidiol (oral intake)
THC Effect on Diclofenac Concentrations CYP2C9
THC Effect on Omeprazole Concentrations on CYP3A4
CBD Effect on Omeprazole Concentrations CYP2C19
THC Effect on Omeprazole Concentrations on CYP2D6
THC Effect on Omeprazole Concentrations CYP2C19
CBD Effect on Diclofenac Concentrations CYP2C9
CBD Effect on Dextromethoprhan Concentrations CYP2D6
CBD Effect on Testosterone Concentrations CYP3A4
Irinotecan PK Â± medicinal cannabis
Docetaxel PK Â± medicinal cannabis
Jar: CBD-Mitoxantrone
BeWo: CBD-mitoxantrone
MCF7/P-gp: CBD-mitoxantrone
Calcein-AM-THC
Rh-123-THC
Plasma CBD Concentrations
Cannabis bulk plant Characterization of Material
Recombinant: CBN-dextromethorphan
Recombinant: CBD-AMMC
Recombinant: CBN-AMMC

pHLM: CBD-dextromethorphan
Recombinant: CBDD-AMMC
Recombinant: THC-dextramethorphan
Recombinant: CBDV-AMMC
HLMs: THC-dextromethorphan
pHLM: CBN-dextromethorphan
Recombinant: CBD-dextromethorphan
Recombinant: THC-AMMC
Recombinant: CBDM-AMMC
CYP3A4-THC
CYP3A4-CBN
CYP3A4-CBD
HLM-THC
HLM-CBN
HLM-CBD
CBD
THC
Induction of CYP1A1 mRNA expression by 50 ÂµM cannabidiol
Non-induction of CYP1A1 mRNA expression by 50 ÂµM cannabinol
Induction of CYP1A1 mRNA expression by 50 ÂµM delta-9-THC
Mitoxantrone-THC
Mitoxantrone-CBN
Mitoxantrone-CBD
Cannabis extract (Cannabidiol) Characterization of Material
NFV+THC PK at Baseline and Day 14
IDV+THC PK at Baseline and Day 14
Inhibition of 11-hydroxylation of delta-8-THC by sulfaphenazole
Weak Inhibition of 7-alpha-hydroxylation of delta-8-THC by sulfaphenazole
Inhibition of 11-hydroxylation of cannabinol by sulfaphenazole
Weak Inhibition of 11-hydroxylation of delta-9-THC by ketoconazole
No inhibition of 7-alpha-hydroxylation of delta-8-THC by 7,8-benzoflavone
Inhibition of 8-hydroxylation of cannabinol by ketoconazole
Weak Inhibition of 11-hydroxylation of delta-9-THC by 7,8-benzoflavone
Inhibition of 7-alpha-hydroxylation of delta-8-THC by ketoconazole
Weak Inhibition of 11-hydroxylation of delta-8-THC by ketoconazole
Inhibition of 11-hydroxylation of delta-9-THC by sulfaphenazole
Inhibition of 8-beta-hydroxylation of delta-9-THC by ketoconazole
Weak Inhibition of 11-hydroxylation of delta-8-THC by 7,8-benzoflavone
No inhibition of 8-beta-hydroxylation of delta-9-THC by 7,8-benzoflavone
Weak Inhibition of 8-hydroxylation of cannabinol by sulfaphenazole
No Inhibition of 8-hydroxylation of cannabinol by 7,8-benzoflavone
Weak Inhibition of 11-hydroxylation of cannabinol by ketoconazole
Weak Inhibition of 11-hydroxylation of cannabinol by 7,8-benzoflavone
Weak Inhibition of 8-beta-hydroxylation of delta-9-THC by sulfaphenazole
CBD Effect on N-desmethylclobazam Concentrations
Stiripentol Effect on CBD, 6-OH-CBD, and 7-COOH-CBD
Clobazam Effect on CBD

CBD Effect on Stiripentol Concentrations
Clobazam Effect on 7-OH-CBD
Stiripentol Effect on 7-OH-CBD
Valproic Acid Effect on Cannabidiol Metabolites
Valproic Acid Effect on CBD
CBD Effect on Midazolam
CBD effect on CLB and N-desmethylclobazam
CBD Effect on Valproic Acid Concentrations
CBD Effect on clobazam and N-desmethylclobazam
Clobazam Effect on 6-OH-CBD
Clobazam Effect on 7-COOH-CBD
CBN-UGT1A9
THC-OH-UGT1A10
THC-COOH-UGT1A3
THC-COOH-UGT1A1
CBN-UGT1A10
THC-OH-UGT1A9
CBN-UGT1A7
CBN-UGT1A8
Increased Clobazam with Cannabidiol (8 weeks)
Increased Clobazam with Cannabidiol (4 weeks)
CBD-Rh123 (Flow-Cytometry Assay)
Cannabidiol-2',6'-dimethyl ether
Cannabidiol
Cannabidiol-2'-monomethyl ether
THC
Cannabidvarin
Decreased systemic exposure of Theophylline with Smoked Tobacco (no Marihuana smoker)
Decreased systemic exposure of Theophylline with Smoked Marihuana (non Tobacco smoker)
Decreased systemic exposure of Theophylline with Smoked Marihuana (Tobacco smoker)
Plasma Concentration of 11-OH-THC when Fed
Plasma Concentration of 11-OH-THC when Fasting
Plasma Concentration of CBD when Fasting
Plasma Concentration of THC when Fasting
Plasma Concentration of THC when Fed
Plasma Concentration of CBD when Fed
CBN on ethanol glucuronidation
CBD-UGT1A9 Inhibition
CBD-UGT2B7 Inhibition
CBD on ethanol glucuronidation
CBN-UGT2B7 Induction
CBN-UGT1A9 Inhibition
rCYP2C9: THC-warfarin
rCYP2C9: THC-diclofenac
iHLMs: CBD-warfarin
iHLM: CBD-diclofenac
iHLM: THC-diclofenac

pHLM: THC-warfarin
rCYP2C9: CBN-diclofenac
rCYP2C9: CBD-diclofenac
pHLM: CBN-warfarin
rCYP2C9: CBD-warfarin
iHLM: CBN-diclofenac
iHLM: THC-warfarin
rCYP2C9: CBN-warfarin
pHLM: CBD-warfarin
iHLM: CBN-warfarin
1A1: THC
HLMs: CBD
HLMs: THC
1A2: THC
1A2: CBD
1A1: CBD
1A2: CBN
1A1: CBN
HLMs: CBN
Secobarbital Plasma Concentrations Following Sodium Secobarbital Ingestion and 150 Âµg/kg CBD Pretreatment
Secobarbital Plasma Concentrations Following Sodium Secobarbital Ingestion and 500 Âµg/kg CBD Pretreatment
Plasma Concentrations of Secobarbital After Placebo Pretreatment and Oral Administration of Secobarbital
Cannabidiol
Cannbidiol-2'-monomethyl ether
CBD-dimethyl ether
Cannabidivarin
6-alpha-OH-CBD-omeprazole
6-alpha-OH-CBD-ketoconazole
6-alpha-OH-CBD-quinidine
6-alpha-OH-CBD-sulfaphenazole
Effect of naltrexone on THC concentration

Experiment type name	Overall effect
In Vitro Enzyme Kinetics	In Vitro Detectable Kinetic Metabolism
In Vitro Transporter Induction	In Vitro Transporter Down Regulation
In Vitro Transporter Induction	In Vitro Transporter Down Regulation
In Vitro Transporter Induction	In Vitro Transporter Induction
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Induction	In Vitro Transporter Down Regulation
In Vitro Transporter Induction	In Vitro Transporter Down Regulation
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Induction	In Vitro Transporter Induction
In Vitro Transporter Induction	In Vitro Transporter Induction
In Vitro Transporter Induction	In Vitro Transporter Induction
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Induction	In Vitro Transporter Induction
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Induction	In Vitro Transporter Non-induction
In Vitro Transporter Induction	In Vitro Transporter Induction
Characterization of Material	
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vivo Pharmacokinetics	
In Vitro Transporter Kinetics	In Vitro Transport
In Vitro Transporter Kinetics	In Vitro Transport
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition

In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Non-inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vivo Interaction	PK Interaction - Increased systemic exposure
In Vivo Interaction	PK Interaction - Increased systemic exposure
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vivo Interaction	No Effect (based on bioequivalence limits)
Characterization of Material	
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition

In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Transporter Induction	In Vitro Transporter Induction
In Vitro Transporter Induction	In Vitro Transporter Induction
In Vitro Enzyme Induction	In Vitro Enzyme Induction
In Vitro Enzyme Induction	In Vitro Enzyme Non-induction
In Vitro Enzyme Induction	In Vitro Enzyme Induction
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
Characterization of Material	
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vivo Interaction	PK Interaction - Increased systemic exposure
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)

In Vivo Interaction	PK Interaction - Increased systemic exposure
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	PK Interaction - Decreased systemic exposure
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	PK Interaction - Decreased systemic exposure
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	PK Interaction - Increased systemic exposure
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vitro Enzyme Kinetics	In Vitro Detectable Kinetic Metabolism
In Vitro Enzyme Kinetics	In Vitro Detectable Kinetic Metabolism
In Vitro Enzyme Kinetics	In Vitro Detectable Kinetic Metabolism
In Vitro Enzyme Kinetics	In Vitro Detectable Kinetic Metabolism
In Vitro Enzyme Kinetics	In Vitro Detectable Kinetic Metabolism
In Vitro Enzyme Kinetics	In Vitro Detectable Kinetic Metabolism
In Vitro Enzyme Kinetics	In Vitro Detectable Kinetic Metabolism
In Vitro Enzyme Kinetics	In Vitro Detectable Kinetic Metabolism
In Vivo Interaction	PK Interaction - Increased systemic exposure
In Vivo Interaction	PK Interaction - Increased systemic exposure
In Vitro Transporter Inhibition	In Vitro Transporter Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vivo Interaction	PK Interaction - Decreased systemic exposure
In Vivo Interaction	PK Interaction - Increased systemic exposure
In Vivo Interaction	PK Interaction - Decreased systemic exposure
In Vivo Pharmacokinetics	
In Vivo Pharmacokinetics	
In Vivo Pharmacokinetics	
In Vivo Pharmacokinetics	
In Vivo Pharmacokinetics	
In Vivo Pharmacokinetics	
In Vitro Enzyme Induction	In Vitro Enzyme Induction
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Induction	In Vitro Enzyme Induction
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition

In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vivo Interaction	No Effect (based on bioequivalence limits)
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition	In Vitro Enzyme Negligible Inhibition
In Vivo Interaction	No Effect (based on bioequivalence limits)

Object compound name

delta-9-tetrahydrocannabinol

3,3â€²-diethyloxacarbocyanine iodide

calcein-am

rhodamine 123

calcein-am

delta-9-tetrahydrocannabinol
delta-9-tetrahydrocannabinol
delta-9-tetrahydrocannabinol
mephenytoin, (s)-
omeprazole
mephenytoin, (s)-
mephenytoin, (s)-
vincristine
fluo3
fluo3
vincristine
fluo3
vincristine

cannabidiol
delta-9-tetrahydrocannabinol
3-o-methylfluorescein
omeprazole
omeprazole
mephenytoin, (s)-
3-o-methylfluorescein
3-o-methylfluorescein
mephenytoin, (s)-
mephenytoin, (s)-

omeprazole
3-o-methylfluorescein
mephenytoin, (s)-
omeprazole
mephenytoin, (s)-
omeprazole
3-o-methylfluorescein
omeprazole
mephenytoin, (s)-
3-o-methylfluorescein
rhodamine 123
rhodamine 123
rhodamine 123
rhodamine 123
rhodamine 123
rhodamine 123
oseltamivir phosphate
oseltamivir phosphate
oseltamivir phosphate
oseltamivir phosphate
oseltamivir phosphate
oseltamivir phosphate
oseltamivir phosphate
oseltamivir phosphate
oseltamivir phosphate
hexobarbital
hexobarbital
diclofenac
testosterone
omeprazole
dextromethorphan
omeprazole
diclofenac
dextromethorphan
testosterone
irinotecan
docetaxel
mitoxantrone
mitoxantrone
mitoxantrone
calcein-am
rhodamine 123
fentanyl

dextromethorphan
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-methoxy-4-methylcoumarin
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-methoxy-4-methylcoumarin

dextromethorphan
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-methoxy-4-methylcoumarin
dextromethorphan
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-methoxy-4-methylcoumarin
dextromethorphan
dextromethorphan
dextromethorphan
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-methoxy-4-methylcoumarin
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-methoxy-4-methylcoumarin
diltiazem
diltiazem
diltiazem
diltiazem
diltiazem
diltiazem

mitoxantrone
mitoxantrone
mitoxantrone

nelfinavir
indinavir
delta-8-tetrahydrocannabinol
delta-8-tetrahydrocannabinol
cannabinol
delta-9-tetrahydrocannabinol
delta-8-tetrahydrocannabinol
cannabinol
delta-9-tetrahydrocannabinol
delta-8-tetrahydrocannabinol
delta-8-tetrahydrocannabinol
delta-9-tetrahydrocannabinol
delta-9-tetrahydrocannabinol
delta-8-tetrahydrocannabinol
delta-9-tetrahydrocannabinol
cannabinol
cannabinol
cannabinol
cannabinol
delta-9-tetrahydrocannabinol
n-desmethylclobazam
cannabidiol
cannabidiol

stiripentol
7-hydroxycannabidiol
7-hydroxycannabidiol
cannabidiol
cannabidiol
midazolam
clobazam
valproic acid
clobazam
6Î±-oh-cannabidiol
7-cooh-cbd
cannabinol
11-hydroxy-delta-9-tetrahydrocannabinol
11-nor-9-carboxy-delta9-tetrahydrocannabinol
11-nor-9-carboxy-delta9-tetrahydrocannabinol
cannabinol
11-hydroxy-delta-9-tetrahydrocannabinol
cannabinol
cannabinol
clobazam
clobazam
rhodamine 123
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
theophylline
theophylline
theophylline

ethanol
ethanol
ethanol

ethanol
(s)-warfarin
diclofenac
(s)-warfarin
diclofenac
diclofenac

(s)-warfarin
diclofenac
diclofenac
(s)-warfarin
(s)-warfarin
diclofenac
(s)-warfarin
(s)-warfarin
(s)-warfarin
(s)-warfarin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
secobarbital
secobarbital
secobarbital
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
7-ethoxyresorufin
cannabidiol
cannabidiol
cannabidiol
cannabidiol
delta-9-tetrahydrocannabinol

Object metabolite compound name

11-hydroxy-delta-9-tetrahydrocannabinol

4-hydroxymephenytoin, (s)-
5-hydroxyomeprazole
4-hydroxymephenytoin, (s)-
4-hydroxymephenytoin, (s)-

fluorescein
5-hydroxyomeprazole
5-hydroxyomeprazole
4-hydroxymephenytoin, (s)-
fluorescein
fluorescein
4-hydroxymephenytoin, (s)-
4-hydroxymephenytoin, (s)-

5-hydroxyomeprazole
fluorescein
4-hydroxymephenytoin, (s)-
5-hydroxyomeprazole
4-hydroxymephenytoin, (s)-
5-hydroxyomeprazole
fluorescein
5-hydroxyomeprazole
4-hydroxymephenytoin, (s)-
fluorescein

oseltamivir acid
oseltamivir acid
oseltamivir acid
oseltamivir acid
oseltamivir acid
oseltamivir acid
oseltamivir acid
oseltamivir acid
oseltamivir acid

4'-hydroxydiclofenac
6beta-hydroxytestosterone
5-hydroxyomeprazole
dextrorphan
5-hydroxyomeprazole
4'-hydroxydiclofenac
dextrorphan
6beta-hydroxytestosterone

dextrorphan
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-hydroxy-4-methylcoumarin
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-hydroxy-4-methylcoumarin

dextrorphan
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-hydroxy-4-methylcoumarin
dextrorphan
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-hydroxy-4-methylcoumarin
dextrorphan
dextrorphan
dextrorphan
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-hydroxy-4-methylcoumarin
3-[2-(n,n-diethyl-n-methylammonium)ethyl]-7-hydroxy-4-methylcoumarin
n-demethyldiltiazem
n-demethyldiltiazem
n-demethyldiltiazem
n-demethyldiltiazem
n-demethyldiltiazem
n-demethyldiltiazem

11-hydroxy-delta-8-tetrahydrocannabinol
7-alpha-hydroxy-delta-8-tetrahydrocannabinol
11-hydroxycannabinol
11-hydroxy-delta-9-tetrahydrocannabinol
7-alpha-hydroxy-delta-8-tetrahydrocannabinol
8-hydroxycannabinol
11-hydroxy-delta-9-tetrahydrocannabinol
7-alpha-hydroxy-delta-8-tetrahydrocannabinol
11-hydroxy-delta-8-tetrahydrocannabinol
11-hydroxy-delta-9-tetrahydrocannabinol
8-beta-hydroxy-delta-9-tetrahydrocannabinol
11-hydroxy-delta-8-tetrahydrocannabinol
8-beta-hydroxy-delta-9-tetrahydrocannabinol
8-hydroxycannabinol
8-hydroxycannabinol
11-hydroxycannabinol
11-hydroxycannabinol
8-beta-hydroxy-delta-9-tetrahydrocannabinol

11-hydroxycannabinol
11-nor-9-carboxy-delta9-tetrahydrocannabinol
glucuronide
glucuronide
11-hydroxycannabinol
11-nor-9-carboxy-delta9-tetrahydrocannabinol
11-hydroxycannabinol
11-hydroxycannabinol

resorufin
resorufin
resorufin
resorufin
resorufin

ethyl glucuronide
ethyl glucuronide
ethyl glucuronide

ethyl glucuronide
7-hydroxywarfarin
4'-hydroxydiclofenac
7-hydroxywarfarin
4'-hydroxydiclofenac
4'-hydroxydiclofenac

7-hydroxywarfarin
4'-hydroxydiclofenac
4'-hydroxydiclofenac
7-hydroxywarfarin
7-hydroxywarfarin
4'-hydroxydiclofenac
7-hydroxywarfarin
7-hydroxywarfarin
7-hydroxywarfarin
7-hydroxywarfarin
resorufin
resorufin
resorufin
resorufin
resorufin
resorufin
resorufin
resorufin
resorufin

resorufin
resorufin
resorufin
resorufin
6Î±-oh-cannabidiol
6Î±-oh-cannabidiol
6Î±-oh-cannabidiol
6Î±-oh-cannabidiol

Precipitant compound name	Enzyme name	Transporter name	Control data
	CYP2C9		FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol		BCRP (ABCG2)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol		BCRP (ABCG2)	FALSE
cannabidiol		BCRP (ABCG2)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol		BCRP (ABCG2)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol		BCRP (ABCG2)	FALSE
cannabidiol		BCRP (ABCG2)	FALSE
			FALSE
ethanol			FALSE
placebo			FALSE
ethanol			FALSE
cannabidiol	CYP2C19		FALSE
cannabidiol	CYP2C19		FALSE
cannabidiol	CYP2C19		FALSE
cannabidiol	CYP2C19		FALSE
cannabinol		ABCC1	FALSE
cannabinol		ABCC1	FALSE
delta-9-tetrahydrocannabinol		ABCC1	FALSE
cannabidiol		ABCC1	FALSE
cannabidiol		ABCC1	FALSE
delta-9-tetrahydrocannabinol		ABCC1	FALSE
			FALSE
		P-gp (ABCB1)	FALSE
		P-gp (ABCB1)	FALSE
delta-9-tetrahydrocannabinol	CYP2C19		FALSE
8,9-dihydrocannabidiol	CYP2C19		FALSE
cannabidivarin	CYP2C19		FALSE
cannabidiol-dimethyl ether	CYP2C19		FALSE
cannabidiol-dimethyl ether	CYP2C19		FALSE
8,9-dihydrocannabidiol	CYP2C19		FALSE
8,9-dihydrocannabidiol	CYP2C19		FALSE
cannabidiol	CYP2C19		FALSE

delta-9-tetrahydrocannabinol	CYP2C19		FALSE
cannabidiol	CYP2C19		FALSE
delta-9-tetrahydrocannabinol	CYP2C19		FALSE
cannabidiol	CYP2C19		FALSE
cannabidivarin	CYP2C19		FALSE
cannabidiol-dimethyl ether	CYP2C19		FALSE
cannabidiol-2'-monomethyl ether	CYP2C19		FALSE
cannabidiol-2'-monomethyl ether	CYP2C19		FALSE
cannabidiol-2'-monomethyl ether	CYP2C19		FALSE
cannabidivarin	CYP2C19		FALSE
delta-9-tetrahydrocannabinol		P-gp (ABCB1)	FALSE
cannabinol		P-gp (ABCB1)	FALSE
cannabinol		P-gp (ABCB1)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
delta-9-tetrahydrocannabinol		P-gp (ABCB1)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabinol	CES1		FALSE
cannabinol	CES1		FALSE
delta-9-tetrahydrocannabinol	CES1		FALSE
cannabidiol	CES1		FALSE
delta-9-tetrahydrocannabinol	CES1		FALSE
cannabidiol	CES1		FALSE
cannabinol	CES1		FALSE
cannabidiol	CES1		FALSE
delta-9-tetrahydrocannabinol	CES1		FALSE
cannabidiol			FALSE
cannabidiol			FALSE
delta-9-tetrahydrocannabinol	CYP2C9		FALSE
delta-9-tetrahydrocannabinol	CYP3A4		FALSE
cannabidiol	CYP2C19		FALSE
delta-9-tetrahydrocannabinol	CYP2D6		FALSE
delta-9-tetrahydrocannabinol	CYP2C19		FALSE
cannabidiol	CYP2C9		FALSE
cannabidiol	CYP2D6		FALSE
cannabidiol	CYP3A4		FALSE
medicinal cannabis	CYP3A		FALSE
medicinal cannabis	CYP3A		FALSE
cannabidiol		BCRP (ABCG2)	FALSE
cannabidiol		BCRP (ABCG2)	FALSE
cannabidiol		P-gp (ABCB1)	FALSE
delta-9-tetrahydrocannabinol		P-gp (ABCB1)	FALSE
delta-9-tetrahydrocannabinol		P-gp (ABCB1)	FALSE
cannabidiol			FALSE
			FALSE
cannabinol	CYP2D6		FALSE
cannabidiol	CYP2D6		FALSE
cannabinol	CYP2D6		FALSE

cannabidiol	CYP2D6		FALSE
cannabidiol-dimethyl ether	CYP2D6		FALSE
delta-9-tetrahydrocannabinol	CYP2D6		FALSE
cannabidivarin	CYP2D6		FALSE
delta-9-tetrahydrocannabinol	CYP2D6		FALSE
cannabinol	CYP2D6		FALSE
cannabidiol	CYP2D6		FALSE
delta-9-tetrahydrocannabinol	CYP2D6		FALSE
cannabidiol-dimethyl ether	CYP2D6		FALSE
delta-9-tetrahydrocannabinol	CYP3A4		FALSE
cannabinol	CYP3A4		FALSE
cannabidiol	CYP3A4		FALSE
delta-9-tetrahydrocannabinol	CYP3A		FALSE
cannabinol	CYP3A		FALSE
cannabidiol	CYP3A		FALSE
cannabidiol		P-gp (ABCB1)	FALSE
delta-9-tetrahydrocannabinol		P-gp (ABCB1)	FALSE
cannabidiol	CYP1A1		FALSE
cannabinol	CYP1A1		FALSE
delta-9-tetrahydrocannabinol	CYP1A1		FALSE
delta-9-tetrahydrocannabinol		BCRP (ABCG2)	FALSE
cannabinol		BCRP (ABCG2)	FALSE
cannabidiol		BCRP (ABCG2)	FALSE
			FALSE
delta-9-tetrahydrocannabinol			FALSE
delta-9-tetrahydrocannabinol			FALSE
sulfaphenazole	CYP2C		FALSE
sulfaphenazole	CYP2C		FALSE
sulfaphenazole	CYP2C		FALSE
ketoconazole	CYP3A		FALSE
alpha-naphthoflavone	CYP1A		FALSE
ketoconazole	CYP3A		FALSE
alpha-naphthoflavone	CYP1A		FALSE
ketoconazole	CYP3A		FALSE
ketoconazole	CYP3A		FALSE
sulfaphenazole	CYP2C		FALSE
ketoconazole	CYP3A		FALSE
alpha-naphthoflavone	CYP1A		FALSE
alpha-naphthoflavone	CYP1A		FALSE
sulfaphenazole	CYP2C		FALSE
alpha-naphthoflavone	CYP1A		FALSE
ketoconazole	CYP3A		FALSE
alpha-naphthoflavone	CYP1A		FALSE
sulfaphenazole	CYP2C		FALSE
cannabidiol			FALSE
stiripentol			FALSE
clobazam			FALSE

cannabidiol			FALSE
clobazam			FALSE
stiripentol			FALSE
valproic acid			FALSE
valproic acid			FALSE
cannabidiol			FALSE
cannabidiol			FALSE
cannabidiol			FALSE
cannabidiol			FALSE
clobazam			FALSE
clobazam			FALSE
	UGT1A9		FALSE
	UGT1A10		FALSE
	UGT1A3		FALSE
	UGT1A1		FALSE
	UGT1A10		FALSE
	UGT1A9		FALSE
	UGT1A7		FALSE
	UGT1A8		FALSE
cannabidiol	CYP3A4		FALSE
cannabidiol			FALSE
cannabidiol		P-gp (ABCB1)	FALSE
cannabidiol-dimethyl ether	CYP1A1		FALSE
cannabidiol	CYP1A1		FALSE
cannabidiol-2'-monomethyl ether	CYP1A1		FALSE
delta-9-tetrahydrocannabinol	CYP1A1		FALSE
cannabidivarin	CYP1A1		FALSE
medicinal cannabis			FALSE
medicinal cannabis			FALSE
medicinal cannabis			FALSE
			FALSE
			FALSE
			FALSE
			FALSE
			FALSE
			FALSE
			FALSE
cannabinol	UGT		FALSE
cannabidiol	UGT1A9		FALSE
cannabidiol	UGT2B7		FALSE
cannabidiol	UGT		FALSE
cannabinol	UGT2B7		FALSE
cannabinol	UGT1A9		FALSE
delta-9-tetrahydrocannabinol	CYP2C9		FALSE
delta-9-tetrahydrocannabinol	CYP2C9		FALSE
cannabidiol	CYP2C9		FALSE
cannabidiol	CYP2C9		FALSE
delta-9-tetrahydrocannabinol	CYP2C9		FALSE

delta-9-tetrahydrocannabinol	CYP2C9	FALSE
cannabinol	CYP2C9	FALSE
cannabidiol	CYP2C9	FALSE
cannabinol	CYP2C9	FALSE
cannabidiol	CYP2C9	FALSE
cannabinol	CYP2C9	FALSE
delta-9-tetrahydrocannabinol	CYP2C9	FALSE
cannabinol	CYP2C9	FALSE
cannabidiol	CYP2C9	FALSE
cannabinol	CYP2C9	FALSE
delta-9-tetrahydrocannabinol	CYP1A1	FALSE
cannabidiol	CYP1A1	FALSE
delta-9-tetrahydrocannabinol	CYP1A1	FALSE
delta-9-tetrahydrocannabinol	CYP1A2	FALSE
cannabidiol	CYP1A2	FALSE
cannabidiol	CYP1A1	FALSE
cannabinol	CYP1A2	FALSE
cannabinol	CYP1A1	FALSE
cannabinol	CYP1A1	FALSE
delta-9-tetrahydrocannabinol		FALSE
delta-9-tetrahydrocannabinol		FALSE
placebo		FALSE
cannabidiol	CYP1A1	FALSE
cannabidiol-2'-monomethyl ether	CYP1A1	FALSE
cannabidiol-dimethyl ether	CYP1A1	FALSE
cannabidivarin	CYP1A1	FALSE
omeprazole	CYP2C19	FALSE
ketoconazole	CYP3A4	FALSE
quinidine	CYP2D6	FALSE
sulfaphenazole	CYP2C9	FALSE
naltrexone		FALSE

Test system name	IC50 shift data
Pooled human liver microsomes	FALSE
BeWo	FALSE
Jar	FALSE
BeWo	FALSE
BeWo	FALSE
BeWo	FALSE
Jar	FALSE
BeWo	FALSE
Jar	FALSE
BeWo	FALSE
MCF7/P-gp	FALSE
MCF7/P-gp	FALSE
Jar	FALSE
BeWo	FALSE
MCF7/P-gp	FALSE
Jar	FALSE
	FALSE
	FALSE
	FALSE
	FALSE
Pooled human liver microsomes	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Pooled human liver microsomes	FALSE
Human ovarian carcinoma cell line	FALSE
Human ABCC1 transduced subline (MRP1)	FALSE
Human ABCC1 transduced subline (MRP1)	FALSE
Human ovarian carcinoma cell line	FALSE
Human ABCC1 transduced subline (MRP1)	FALSE
Human ovarian carcinoma cell line	FALSE
	FALSE
Caco-2 cells	FALSE
Caco-2 cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
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Baculovirus-insect cells	FALSE
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Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Other cells	FALSE
Other cells	FALSE
Other cells	FALSE
Other cells	FALSE
Other cells	FALSE
Other cells	FALSE
Human kidney S9 fraction	FALSE
Human kidney S9 fraction	FALSE
Human kidney S9 fraction	FALSE
Human kidney S9 fraction	FALSE
Human kidney S9 fraction	FALSE
Human kidney S9 fraction	FALSE
Human kidney S9 fraction	FALSE
Human kidney S9 fraction	FALSE
Human kidney S9 fraction	FALSE
	FALSE
	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
	FALSE
	FALSE
Jar	FALSE
BeWo	FALSE
MCF7/P-gp	FALSE
HEK293 transfected cells	FALSE
HEK293 transfected cells	FALSE
	FALSE
	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Pooled human liver microsomes	FALSE

Pooled human liver microsomes	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Individual human liver microsomes	FALSE
Individual human liver microsomes	FALSE
Individual human liver microsomes	FALSE
Other cells	FALSE
Other cells	FALSE
HepG2 cell line	FALSE
HepG2 cell line	FALSE
HepG2 cell line	FALSE
Other cells	FALSE
Other cells	FALSE
Other cells	FALSE
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Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
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Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
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LLC-PK1 transfected cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
	FALSE
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	FALSE
Human cryopreserved hepatocytes	FALSE
Human cryopreserved hepatocytes	FALSE
Human cryopreserved hepatocytes	FALSE
Human cryopreserved hepatocytes	FALSE
Human cryopreserved hepatocytes	FALSE
Human cryopreserved hepatocytes	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Individual human liver microsomes	FALSE
Individual human liver microsomes	FALSE
Individual human liver microsomes	FALSE

Pooled human liver microsomes	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Pooled human liver microsomes	FALSE
Baculovirus-insect cells	FALSE
Individual human liver microsomes	FALSE
Individual human liver microsomes	FALSE
Baculovirus-insect cells	FALSE
Pooled human liver microsomes	FALSE
Individual human liver microsomes	FALSE
Baculovirus-insect cells	FALSE
Pooled human liver microsomes	FALSE
Pooled human liver microsomes	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Pooled human liver microsomes	FALSE
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Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
Baculovirus-insect cells	FALSE
	FALSE

Research organization's overall effect cutoff

N/A
N/A
N/A
N/A
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N/A
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N/A
NA
Not provided. A common convention is that IC50 > 100 micM signals negligible inhibition
Not provided. A common convention is that IC50 > 100 micM signals negligible inhibition
NA
Not provided. A common convention is that IC50 > 100 micM signals negligible inhibition
Not provided. A common convention is that IC50 > 100 micM signals negligible inhibition

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90% inhibition
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90% inhibition
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"The mean accumulation index had to be significantly > 1 ($p<0.05$) to assess transporter inhibition potency by flow
"The mean accumulation index had to be significantly > 1 ($p < 0.05$) to assess transporter inhibition potency by flov

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"The significance of differences between the means of the various groups was evaluated by means of a one-way ar
"The significance of differences between the means of the various groups was evaluated by means of a one-way ar
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Inhibition of Rh123 efflux caused by the treatment of 5 Î¼M PSC833 was defined as 100% inhibition
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Research organization's experiment ID

cyotmetry (n = 3 minimum)"
ɴ cytometry (n = 3 minimum)."

nalysis of variance followed by Bonferroni or
nalysis of variance followed by Bonferroni or
nalysis of variance followed by Bonferroni or

1102

GWEP1543

GWEP1543
GWEP1543
GWEP17028
GWEP1543
GWEP1543
GWEP1428

Additional information

Table 1

Figure 2
Figure 2Placebo is orange juice sprayed with 100-proof vodka
Figure 2

As per Table 3.Two-compartment linear model with zero-order absorption.Diphenhydramine was used a positive c

Acute T lymphoblastoid leukaemia cell line
Acute T lymphoblastoid leukaemia cell line (CCRF-CEM)
CEM/VLB100 cell line (multidrug resistant sub line)
Acute T lymphoblastoid leukaemia cell line
CEM/VLB100 cell line (multidrug resistant sub line)
CEM/VLB100 cell line (multidrug resistant sub line)

Table 2
Table 3

(Figure 2)

CEM/VLB100 cell line
CEM/VLB100 cell-line used
Dunnett's post-hoc test."
Dunnett's post-hoc test."
Dunnett's post-hoc test."

NFV = nelfinavirTHC = delta-9-THC
IDV = indiavirTHC = delta-9-THCBaseline = controlDay 14 = test

From page 109 of "Clinical Pharmacology Biopharmaceutics Review"
Study GWEP1543
Study GWEP1543

Study GWEP1543
Study GWEP1543
Study GWEP1543
Study GWEP1543
Study GWEP1543
Systemic exposure to midazolam was relatively unaffected by concomitant administration of CBD indicating lack of
Study GWEP1543
Study GWEP1543
Study GWEP1428 (p 106)
Study GWEP1543
Study GWEP1543
Table 2
Table 2
Table 2

Table 2

Table 2
Table 2

Table 1This studies the active metabolite of THC
Table 1This studies the active metabolite of THC
Table 1
Table 1
Table 1
(Table 1)

Figure 1
Figure 1
Table 1.

Cytochrome b5 purchased but no mention of how used in the study
(Table 2)

Experimental conditions comment

Blood samples drawn at described times after the beginning of ethanol administration

incubation time with two phases, cells and natural products for 30 min and then with Vincristine for another 90 mi
â€œincubation time with two phases, cells and natural products for 30 min and then with Fluo3 for another 60 mi
â€œincubation time with two phases, cells and natural products for 30 min and then with Fluo3 for another 60 mi
incubation time with two phases, cells and natural products for 30 min and then with Vincristine for another 90 mi
incubation time with two phases, cells and natural products for 30 min and then with Fluo3 for another 60 min.
incubation time with two phases, cells and natural products for 30 min and then with Vincristine for another 90 mi
ontrol.

CYP cocktail: Diclofenac (CYP2C9, 5 ÂµM), dextromethorphan (CYP2D6, 5 ÂµM), omeprazole (CYP2C19, 10 ÂµM) a

CYP cocktail: Diclofenac (CYP2C9, 5 ÂµM), dextromethorphan (CYP2D6, 5 ÂµM), omeprazole (CYP2C19, 10 ÂµM) a
CYP cocktail: Diclofenac (CYP2C9, 5 ÂµM), dextromethorphan (CYP2D6, 5 ÂµM), omeprazole (CYP2C19, 10 ÂµM) a
CYP cocktail: Diclofenac (CYP2C9, 5 ÂµM), dextromethorphan (CYP2D6, 5 ÂµM), omeprazole (CYP2C19, 10 ÂµM) a

Biphasic with at least one week interim.(Figure 1)
Moisture content: 10.5 Â± 0.16% (n = 3) by gravimetric measurement.

Heavy metals analysis have been done by ICP-MS, loss on drying analysis have been done by IR radiation.

Inclusion criteria: at least 18 years old, have documented HIV infection, and be on a stable antire- troviral treatme

f inhibition or induction of CYP3A4. The increased exposure to 1'-hydroxymidazolam may be due to downstream in

Patients began taking CBD at a dose of 5 mg/kg/day and titrated up by 5 mg/kg/day each week to a goal of 25 mg/

(Table 1, Study 2b)

Experimental results comment

Table 1. Vmax converted from pmol/min/mg to nmol/min/mg [463 (15) pmol/min mg protein]
figure 2
figure 3
FIGURE 2
the accumulation measurement is intracellular accumulation as measured by fluorescence

figure 5
the accumulation measurement is intracellular accumulation as measured by fluorescence
FIGURE 3
figure 5
figure 4
the accumulation measurement is intracellular accumulation as measured by fluorescence
figure 3
the accumulation measurement is intracellular accumulation as measured by fluorescence
figure 4
figure 5
Heavy metals (Pb, Hg, Cd and As) were not detected, as well as Aflatoxins B1, B2, G1 and G2.
Values converted from minutes.Â Original values: Time to peak (min): 5.7 Â± 0.7 AUC0-315Â (ng*min/mL): 3792Â Â
Values converted from minutes.Original values: Time to peak (min): 7.2Â Â± 0.7 AUC0-315 (ng*min/mL): 3695Â Â±
Values converted from minutes.Â Original values: Time to peak (min): 5.8 Â± 1 AUC0-315 (ng*min/mL): 4019Â Â± 5

Measurements show 50% reduction in transport using increase in intracellular accumulation based on % of parent
â€œMeasurements show 50% reduction in transport using increase in intracellular accumulation based on % of pa
â€œMeasurements show 50% reduction in transport using increase in intracellular accumulation based on % of pa
Measurements show 50% reduction in transport using increase in intracellular accumulation based on % of parent
â€œMeasurements show 50% reduction in transport using increase in intracellular accumulation based on % of pa
Measurements show 50% reduction in transport using increase in intracellular accumulation based on % of parent
Table 3. Estimated values
Fig 2. Estimated at 240 min.
Figure 2. Estimated at 240 min.
Table 2
Table 2
Table 2
%inhibition at 50Â Î¼M (Fig 2C).IC50 (Table 2).Ki (Table 3).
Table 2
Table 2
%inhibition at 6Â Î¼M (Fig 2F)IC50 (Table 2)Ki (Table 3)
%inhibition at 10Â Î¼M of CBD (Fig. 1)IC50 (Table 1), Ki (Table 3)

Table 2
Table 2
% inhibition at 10 Î¼M estimated from Fig 2D.IC50 (Table 2).Ki (Table 3)
Table 2
%inhibition at 10Â Î¼M (Fig 2E)IC50 (Table 2)Ki (Table 3)
Table 2
Table 2
Table 2
%inhibition at 10Â Î¼M (Fig.2C)IC50 (Table 2)Ki (Table 3)
Table 2
Table 1.
Table 1
Table 1.Accumulation estimated from Fig 1a at 10Â Î¼M
Table 1.
Table 1.Accumulation estimated from Fig 1c at 10Â Î¼M
Table 1.%inhibition estimated from Fig 1b at 10Â Î¼M
IC50 pre-incubation 0 min (A) = 4.03 ÂµMIC50 pre-incubation 30 min (B) = 8.51 ÂµMB/A = 2.11
IC50 pre-incubation 0 min (A) = 4.03 ÂµMIC50 pre-incubation 30 min (B) = 8.51 ÂµMB/A = 2.11
IC50 pre-incubation 0 min (A) = 3.91 ÂµMIC50 pre-incubation 30 min (A) = 11.2 ÂµMB/A = 2.85
Table 2
Table 2
IC50 pre-incubation 0 min (A) = 7.73 ÂµMIC50 pre-incubation 30 min (B) = 12.1 ÂµMB/A = 1.57
Table 2
IC50 pre-incubation 0 min (A) = 7.73 ÂµMIC50 pre-incubation 30 min (B) = 12.1 ÂµMB/A = 1.57
IC50 pre-incubation 0 min (A) = 3.91 ÂµMIC50 pre-incubation 30 min (B) = 11.2 ÂµMB/A = 2.85

measurement after CBD
MeanÂ±SD of IC50 values with duplicate determinations determined using Log avg [THC]
MeanÂ±SD of IC50 values with duplicate determinations determined using Log avg [THC]
IC50Â log average reported Nominal: 2.8 Â± 1.4 Published: 1.55 Î¼M2
MeanÂ±SD of IC50 values with duplicate determinations determined using Log avg [THC]
MeanÂ±SD of IC50 values with duplicate determinations determined using Log avg [THC]
IC50Â log average reported Nominal: 2.8 Â± 0.7 Published: 5.47 Î¼M2
IC50Â log average reported Nominal: 6.4 Â± 3.6 Published: 4.01 Î¼M2
IC50Â log average reported Nominal: 3.9 Â± 1.5 Published: 9.18 Î¼M2
Table 2.
Table 3.
Fig 1b at 25Â Î¼M CBD10Â Î¼M CBD ~125% Â± 10% inhibitionTable 1
Figure 1a at 25Â Î¼M CBD10Â Î¼M CBD ~130% Â± 15% inhibition
Fig 1c atÂ 20Â Î¼M CBD 10Â Î¼M CBD ~140% Â± 20% inhibitionTable 1
Fig 2a.PSC833 5Â Î¼M was used as a positive control
Fig 2bPSC833 5Â Î¼M was used as a positive control
Value reported estimated at 3 hours with 800 mg CBD (original value reported = ~170 Âµg/L)With 400 mg CBD, Cm
Cannabinoid Content Using Non-derivatized Extracts
Table 1
Table 1Figure 3
Table 1

Table 1Figure 3
Figure 4E
Table 1
Figure 5Figure 4E Ki atÂ log(-4.4) (concentration estimated)
Table 1
Table 1
Table 1Figure 3
Table 1 (AMMC)Table 3 (20 min)
Figure 4C
Table 2
Table 2
Table 2, Table 3
Table 2
Table 2
Table 2, Table 3
Estimated from Fig 1b and 1d. at 4 hr
Emax: Fig 1a. Reported at 4 h.Change from vehicle control: Estimated from Fig 1c. Reported at 4 h.
Figure 2
Estimated from Figure 2
Figure 2
Table 1 (MEF3.8/Bcrp1 A2)
Table 1 (MEF3.8/Bcrp1 A2)
Table 1 (MEF3.8/Bcrp 1 A2)

Table 3. Cmax % change reported -17.4 (-43-64). AUC0-8 % change reported -10.2 (-46-92).
Table 2. Cmax % Change reported as -14.1 (-58 to 7), p = 0.039; AUC0-8 % change reported as -14 (-66 to 44)Despit
Table 1
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Table 1
From page 109Units for these values are NOT means but are instead a ratio of day 33 values:day 1 values

When CBD was combined with stiripentol there was a minor increase in Cmax and AUCtau; 1.28 and 1.55-fold, resp

C estimated from Fig 8; page 111
Clobazam exposure was increased slightly (~20%) by co-administration with CBD while exposure to the n-desmeth

Test ratios indicate the Day33:Day 1 ratio for individuals allocated to active drug.Control ratios indicate the Day 33

Table 2
Table 2
Table 2
Table 2
Table 2
Table 2
Table 2.
Table 2
kg/day. Throughout the study, CLB doses were either kept constant or decreased when side effects were observed.

Accumulation estimated from Fig 3a at 30Â Î¼M of CBD. p < 0.01 versus control%inhibition estimated from Fig 5 at
%inhibition estimated from Fig 3 at 25 Î¼M.Table 1.
Estimated from Fig 4a. CBD 1 Î¼M.Table 1
%inhibition estimated from Fig 3Table 1
Fig 5Table 1
%inhibition estimated from Fig 4a.Table 1

Table 1
Table 1
Table 1
Values from Table 1.The following values are from the fed state (Figure 1a and Table 1):Cmax: 6.2Â Â± 1.3 ng/mLA
Table 1
Results from Table 1
Estimated from Fig 4 at 15 mg/L.

%inhibition estimated from Fig 4 at 15 mg/L.Ki (3.1 mg/L) from Fig 5.IC50 (1.17 mg/L) and Ki converted from mg/L t

Tables 2, 3, and 4IC50 preincubation time recorded at 20 min
Tables 2 and 3
Tables 2 and 3
Tables 2 and 3
Tables 2 and 3

Tables 2, 3, and 4.IC50 pre-incubation recorded at 20 min
Tables 2 and 3
Tables 2 and 3
Tables 2, 3, and 4.IC50 pre-incubation recorded at 20 min
Tables 2, 3, and 4IC50 preincubation time recorded at 20 min
Tables 2 and 3
Tables 2 and 3
Tables 2, 3, and 4IC50 preincubation time recorded at 20 min
Tables 2, 3, and 4.IC50 pre-incubation recorded at 20 min
Tables 2 and 3
Tables 2, 3, and 4IC50 at 20 min
Tables 2 and 3.IC50 at 20 min
Tables 2 and 3.IC50 at 20 min
Tables 2 and 3IC50 at 20 minFig 4. %inhibition estimated for 8Â Î¼M
Tables 2, 3, and 4IC50 at 20 min
Tables 2, 3, and 4.Â IC50 at 20 min.Fig 4. % inhibition estimated with 0.625Â Î¼MFig 5. With NADPH at 9 min
Tables 2 and 3IC50 at 20 min
Tables 2, 3, and 4IC50 at 20 min
Tables 2 and 3.IC50 at 20 min
Values estimated from Figure 1 and converted fromÂ Âµg/mL. Original estimated value: 2.5Â Âµg/mL.
Values estimated from Figure 1. Original value was converted to ng/mL: Cmax (Âµg/mL): 2.75
Values converted fromÂ Âµg/mL.Â Original value: Cmax (Âµg/mL): 2.59 Â± 0.94Table 1.
% inhibition estimated from Figure 2 at 20 min. IC50 at 0 min - 0.671IC50 at 20 min (table 1)Kinact/KI converted frc
%inhibition estimated from Figure 2.IC50pre-incubation at 0 min (Table 1).IC50pre-incubation at 20 min - 1.90Kina
%inhibitionpre-incubation at estimated 50Â Î¼M at 20 min (Figure 2).IC50pre-incubation at 0 min (Table 1)IC50pre
%inhibition estimated from Fig 2 at 20 min, ~0.5Â Î¼M CBDV.IC50 at 0 min (table 1).IC50 at 20 min 0.0677Kinact/K
Table 4 (100-(residual activity (% of control))
Table 4 (100-(residual activity (% of control))
Table 4 (100-(residual activity (% of control))
Table 4 (100-residual activity (% of control))
Table 2. Cmax of control at t = 240 min; Cmax of test at t = 120 min. P value significance extrapolated from stateme

Internal: Additional comments

Â± 530 Figure 2.
: 597 Figure 2.
585 Figure 2

concentration.
rent concentrationâ€
rent concentrationâ€
concentration.
Cell line = human ABCC1 transduced subline (2008/MRP1)
concentration.

ıax mean Â± SEM ~ 140 Âµg/LÂ Â± 20 Âµg/LValues above converte

:e a statistically significant decrease in Cmax of IDV in the marijuan

pectively.

ylclobazam metabolite was increased by 3.4 fold as a result of con

:Day ratio for individuals allocated to placebo.CBD did not alter Cn

. CLB doses were recorded and plasma levels of CLB, nCLB, and CBI

: 100 Î¼M.IC50 found within text

UC(0-inf): 34.99 (16.41) h*ng/mLAUC(0-t): 32.7 (16.75) h*ng/mLCl

toÂ Âµg/mL

ɔm /min/mmol to /min/Î¼M (table 2).All other values from Table 2
ct/KI converted from /min/mmol to /min/Î¼M (table 2).All other v
-incubation at 20 min - 7.68Kinact/KI converted from /min/mmol t
I converted from /min/mmol to /min/Î¼M (table 2).All other value

ɛnt within the text: "Table 2, which portrays plasma levels of D9-TH

Study title
CYP2C-catalyzed delta9-tetrahydrocannabinol metabolism: kinetics, pharmacogenetics and interaction with pheny
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabidiol changes P-gp and BCRP expression in trophoblast cell lines.
Cannabis extract (THC) Characterization of Material
Interaction between Marihuana and Ethanol: Effects on Psychomotor Performance
Interaction between Marihuana and Ethanol: Effects on Psychomotor Performance
Interaction between Marihuana and Ethanol: Effects on Psychomotor Performance
Cannabidiol is a potent inhibitor of the catalytic activity of cytochrome P450 2C19.
Cannabidiol is a potent inhibitor of the catalytic activity of cytochrome P450 2C19.
Cannabidiol is a potent inhibitor of the catalytic activity of cytochrome P450 2C19.
Cannabidiol is a potent inhibitor of the catalytic activity of cytochrome P450 2C19.
Interaction of plant cannabinoids with the multidrug transporter ABCC1 (MRP1)
Interaction of plant cannabinoids with the multidrug transporter ABCC1 (MRP1)
Interaction of plant cannabinoids with the multidrug transporter ABCC1 (MRP1)
Interaction of plant cannabinoids with the multidrug transporter ABCC1 (MRP1)
Interaction of plant cannabinoids with the multidrug transporter ABCC1 (MRP1)
Interaction of plant cannabinoids with the multidrug transporter ABCC1 (MRP1)
Does olanzapine inhibit the psychomimetic effects of Î”9-tetrahydrocannabinol?
Pharmacological Effects of Cannabinoids on the Caco-2 Cell Culture Model of Intestinal Permeability
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Cannabidiol Is a Potent Inhibitor of the Catalytic Activity of Cytochrome P450 2C19
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The effects of cannabinoids on P-glycoprotein transport and expression in multidrug resistant cells.
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In Vitro Inhibition of Carboxylesterase 1 by Major Cannabinoids and Selected Metabolites
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Metabolic and psychophysiologic studies of cannabidiolhexobarbital interaction
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Cannabinoids as perpetrators of drug interactions - Using in vitro data to inform clinical study design
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Medicinal Cannabis Does Not Influence the Clinical Pharmacokinetics of Irinotecan and Docetaxel
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Cannabidiol enhances xenobiotic permeability through the human placental barrier by direct inhibition of breast c
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Interaction of drugs of abuse and maintenance treatments with human P-glycoprotein (ABCB1) and breast cancer
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Safety and pharmacokinetics of oral cannabidiol when administered concomitantly with intravenous fentanyl in hu
Cannabis Characterization of Bulk Plant Material
Cannabidiol, a major phytocannabinoid, as a potent atypical inhibitor for CYP2D6.
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Potent inhibition of human cytochrome P450 3A isoforms by cannabidiol: role of phenolic hydroxyl groups in the r

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CB2 and TRPV1 receptors mediate cannabinoid actions on MDR1 expression in multidrug resistant cells

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Cannabidiol induces expression of human cytochrome P450 1A1 that is possibly mediated through aryl hydrocarbo

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The multidrug transporter ABCG2 (BCRP) is inhibited by plant-derived cannabinoids.

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Cannabis extract (CBD) Characterization of Material

The effects of cannabinoids on the pharmacokinetics of indinavir and nelfinavir

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Cytochrome P450 enzymes involved in the metabolism of tetrahydrocannabinols and cannabinol by human hepati

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Drug Approval Package: Epidiolex (Cannabidiol)

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Characterization of Human Hepatic and Extrahepatic UDP-Glucuronosyltransferase Enzymes Involved in the Metab
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Drug-drug interaction between clobazam and cannabidiol in children with refractory epilepsy
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Characterization of P-glycoprotein Inhibition by Major Cannabinoids from Marijuana
Structural requirements for potent direct inhibition of human cytochrome P450 1A1 by cannabidiol: role of pentyl
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Enhanced biotransformation of theophylline in marihuana and tobacco smokers.
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A phase I study to assess the effect of food on the single dose bioavailability of the THC/CBD oromucosal spray
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Involvement of UDP-Glucuronosyltransferases UGT1A9 and UGT2B7 in Ethanol Glucuronidation, and Interactions w
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Comparison in the in vitro inhibitory effects of major phytocannabinoids and polycyclic aromatic hydrocarbons com
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Characterization of major phytocannabinoids, cannabidiol and cannabinol, as isoform-selective and potent inhibitc
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Influence of cannabidiol on secobarbital effects and plasma kinetics
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Characterization of the structural determinants required for potent mechanism-based inhibition of human cytochr
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Identification of cytochrome P450 enzymes responsible for metabolism of cannabidiol by human liver microsomes
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Interaction between naltrexone and oral THC in heavy marijuana smokers

Study URL	NaPDI study ID	Study pubmed ID	Study source type
http://repo.napdi.org/NPDI-0mD33A	PMID: 16112652	16112652	1
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Quantified metabolite name	Quantified metabolite InChI
cannabidiol	QHMBSVQNZZTUGM-ZWKOTPCHSA-N

cannabidiol	QHMBSVQNZZTUGM-ZWKOTPCHSA-N

cannabidiol	QHMBSVQNZZTUGM-ZWKOTPCHSA-N

Object metabolite compound ID	Object metabolite compound InChI
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3	OQPLORUDZLXXPD-UHFFFAOYSA-N
148	CMZHQFXXAAIBKE-UHFFFAOYSA-N
3	OQPLORUDZLXXPD-UHFFFAOYSA-N
3	OQPLORUDZLXXPD-UHFFFAOYSA-N
146	GNBHRKFJIUUOQI-UHFFFAOYSA-N
148	CMZHQFXXAAIBKE-UHFFFAOYSA-N
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3	OQPLORUDZLXXPD-UHFFFAOYSA-N
146	GNBHRKFJIUUOQI-UHFFFAOYSA-N
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148 CMZHQFXXAAIBKE-UHFFFAOYSA-N
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148 CMZHQFXXAAIBKE-UHFFFAOYSA-N
 13 JAQUASYNZVUNQP-PVAVHDDUSA-N
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154 YDKZOUNVEIGJPO-UHFFFAOYSA-N
119 YCBKSSAWEUDACY-IAGOWNOFSA-N
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154 YDKZOUNVEIGJPO-UHFFFAOYSA-N
154 YDKZOUNVEIGJPO-UHFFFAOYSA-N
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154 YDKZOUNVEIGJPO-UHFFFAOYSA-N
124 YOVRGSHRZRJTLZ-HZPDHXFCSA-N
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166 IWJBVMJWSPZNJH-UQGZVRACSA-N
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167 SKFYEJMLNMTTJA-UHFFFAOYSA-N
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157 YYLPAYRRVSQJRR-KSZLIROESA-N
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Object metabolite compound description	Object metabolite compound concept ID (omop)
11-OH-THC	

4349487

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11-OH-THC

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Precipitant compound ID	Precipitant compound international chemical identifier
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125	LFQSCWFLJHTTHZ-UHFFFAOYSA-N
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125	LFQSCWFLJHTTHZ-UHFFFAOYSA-N
115	QHMBSVQNZZTUGM-ZWKOTPCHSA-N
115	QHMBSVQNZZTUGM-ZWKOTPCHSA-N
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153	VBGLYOIFKLUMQG-UHFFFAOYSA-N
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115	QHMBSVQNZZTUGM-ZWKOTPCHSA-N
118	CYQFCXCEBYINGO-UHFFFAOYSA-N
118	CYQFCXCEBYINGO-UHFFFAOYSA-N
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140	UYBGHBAVRNATET-VQTJNVASSA-N
140	UYBGHBAVRNATET-VQTJNVASSA-N
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149	
115	QHMBSVQNZZTUGM-ZWKOTPCHSA-N

118 CYQFCXCEBYINGO-UHFFFAOYSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
118 CYQFCXCEBYINGO-UHFFFAOYSA-N
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140 UYBGHBAVRNATET-VQTJNVASSA-N
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115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
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115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
118 CYQFCXCEBYINGO-UHFFFAOYSA-N
118 CYQFCXCEBYINGO-UHFFFAOYSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N

153 VBGLYOIFKLUMQG-UHFFFAOYSA-N
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153 VBGLYOIFKLUMQG-UHFFFAOYSA-N

115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
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118 CYQFCXCEBYINGO-UHFFFAOYSA-N
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118 CYQFCXCEBYINGO-UHFFFAOYSA-N
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118 CYQFCXCEBYINGO-UHFFFAOYSA-N
118 CYQFCXCEBYINGO-UHFFFAOYSA-N
156 QWCJHSGMANYXCW-UHFFFAOYSA-N
156 QWCJHSGMANYXCW-UHFFFAOYSA-N
156 QWCJHSGMANYXCW-UHFFFAOYSA-N
102 XMAYWYJOQHXEEK-OZXSUGGESA-N
257 VFMMPHCGEFXGIP-UHFFFAOYSA-N
102 XMAYWYJOQHXEEK-OZXSUGGESA-N
257 VFMMPHCGEFXGIP-UHFFFAOYSA-N
102 XMAYWYJOQHXEEK-OZXSUGGESA-N
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156 QWCJHSGMANYXCW-UHFFFAOYSA-N
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257 VFMMPHCGEFXGIP-UHFFFAOYSA-N
257 VFMMPHCGEFXGIP-UHFFFAOYSA-N
156 QWCJHSGMANYXCW-UHFFFAOYSA-N
257 VFMMPHCGEFXGIP-UHFFFAOYSA-N
102 XMAYWYJOQHXEEK-OZXSUGGESA-N
257 VFMMPHCGEFXGIP-UHFFFAOYSA-N
156 QWCJHSGMANYXCW-UHFFFAOYSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
202 IBLNKMRFIPWSOY-FNORWQNLSA-N
200 CXOXHMZGEKVPMT-UHFFFAOYSA-N

115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
200 CXOXHMZGEKVPMT-UHFFFAOYSA-N
202 IBLNKMRFIPWSOY-FNORWQNLSA-N
203 NIJJYAXOARWZEE-UHFFFAOYSA-N
203 NIJJYAXOARWZEE-UHFFFAOYSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
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200 CXOXHMZGEKVPMT-UHFFFAOYSA-N
200 CXOXHMZGEKVPMT-UHFFFAOYSA-N

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140 UYBGHBAVRNATET-VQTJNVASSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
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118 CYQFCXCEBYINGO-UHFFFAOYSA-N
142 REOZWEGFPHTFEI-JKSUJKDBSA-N
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153 VBGLYOIFKLUMQG-UHFFFAOYSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
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115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
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153 VBGLYOIFKLUMQG-UHFFFAOYSA-N
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118 CYQFCXCEBYINGO-UHFFFAOYSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
118 CYQFCXCEBYINGO-UHFFFAOYSA-N

118 CYQFCXCEBYINGO-UHFFFAOYSA-N
153 VBGLYOIFKLUMQG-UHFFFAOYSA-N
115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
153 VBGLYOIFKLUMQG-UHFFFAOYSA-N
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118 CYQFCXCEBYINGO-UHFFFAOYSA-N
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115 QHMBSVQNZZTUGM-ZWKOTPCHSA-N
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140 UYBGHBAVRNATET-VQTJNVASSA-N
142 REOZWEGFPHTFEI-JKSUJKDBSA-N
100 SUBDBMMJDZJVOS-UHFFFAOYSA-N
102 XMAYWYJOQHXEEK-OZXSUGGESA-N
101 LOUPRKONTZGTKE-LHHVKLHASA-N
156 QWCJHSGMANYXCW-UHFFFAOYSA-N
123 DQCKKXVULJGBQN-XFWGSAIBSA-N

Precipitant compound description	Object compound ID
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CBD derivative	25
CBD derivative	150
	150
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	100
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CBD derivative	100
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CBD derivative	108
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CBD derivative	108
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CBD derivative	86
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CBD derivative	86
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	118

Object compound unique ingredient identifier	Object compound InChI
	CYQFCXCEBYINGO-UHFFFAOYSA-N
	FIZZUEJIOKEFFZ-UHFFFAOYSA-M
	XKFSBWQWNMZWFA-UHFFFAOYSA-N
	MYFATKRONKHHQL-UHFFFAOYSA-N
	XKFSBWQWNMZWFA-UHFFFAOYSA-N
	CYQFCXCEBYINGO-UHFFFAOYSA-N
	CYQFCXCEBYINGO-UHFFFAOYSA-N
	CYQFCXCEBYINGO-UHFFFAOYSA-N
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	SUBDBMMJDZJVOS-UHFFFAOYSA-N
D9818430MW	GMHKMTDVRCWUDX-LBPRGKRZSA-N
D9818430MW	GMHKMTDVRCWUDX-LBPRGKRZSA-N
	OGWKCGZFUXNPDA-XQKSVPLYSA-N
	OZLGRUXZXMRXGP-UHFFFAOYSA-N
	OZLGRUXZXMRXGP-UHFFFAOYSA-N
	OGWKCGZFUXNPDA-XQKSVPLYSA-N
	OZLGRUXZXMRXGP-UHFFFAOYSA-N
	OGWKCGZFUXNPDA-XQKSVPLYSA-N
	QHMBSVQNZZTUGM-ZWKOTPCHSA-N
	CYQFCXCEBYINGO-UHFFFAOYSA-N
	KDXNYSZNOWTPLE-UHFFFAOYSA-N
	SUBDBMMJDZJVOS-UHFFFAOYSA-N
	SUBDBMMJDZJVOS-UHFFFAOYSA-N
D9818430MW	GMHKMTDVRCWUDX-LBPRGKRZSA-N
	KDXNYSZNOWTPLE-UHFFFAOYSA-N
	KDXNYSZNOWTPLE-UHFFFAOYSA-N
D9818430MW	GMHKMTDVRCWUDX-LBPRGKRZSA-N
D9818430MW	GMHKMTDVRCWUDX-LBPRGKRZSA-N

	SUBDBMMJDZJVOS-UHFFFAOYSA-N
	KDXNYSZNOWTPLE-UHFFFAOYSA-N
D9818430MW	GMHKMTDVRCWUDX-LBPRGKRZSA-N
	SUBDBMMJDZJVOS-UHFFFAOYSA-N
D9818430MW	GMHKMTDVRCWUDX-LBPRGKRZSA-N
	SUBDBMMJDZJVOS-UHFFFAOYSA-N
	KDXNYSZNOWTPLE-UHFFFAOYSA-N
	SUBDBMMJDZJVOS-UHFFFAOYSA-N
D9818430MW	GMHKMTDVRCWUDX-LBPRGKRZSA-N
	KDXNYSZNOWTPLE-UHFFFAOYSA-N
	MYFATKRONKHHQL-UHFFFAOYSA-N
	MYFATKRONKHHQL-UHFFFAOYSA-N
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	MYFATKRONKHHQL-UHFFFAOYSA-N
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	PGZUMBJQJWIWGJ-ONAKXNSWSA-N
	PGZUMBJQJWIWGJ-ONAKXNSWSA-N
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	MUMGGOZAMZWBJJ-DYKIIFRCSA-N
	SUBDBMMJDZJVOS-UHFFFAOYSA-N
7355X3ROTS	MKXZASYAUGDDCJ-NJAFHUGGSA-N
	SUBDBMMJDZJVOS-UHFFFAOYSA-N
144O8QL0L1	DCOPUUMXTXDBNB-UHFFFAOYSA-N
7355X3ROTS	MKXZASYAUGDDCJ-NJAFHUGGSA-N
	MUMGGOZAMZWBJJ-DYKIIFRCSA-N
	UWKQSNNFCGGAFS-XIFFEERXSA-N
	ZDZOTLJHXYCWBA-VCVYQWHSSA-N
	KKZJGLLVHKMTCM-UHFFFAOYSA-N
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	XKFSBWQWNMZWFA-UHFFFAOYSA-N
	MYFATKRONKHHQL-UHFFFAOYSA-N
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7355X3ROTS MKXZASYAUGDDCJ-NJAFHUGGSA-N

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7355X3ROTS MKXZASYAUGDDCJ-NJAFHUGGSA-N
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KKZJGLLVHKMTCM-UHFFFAOYSA-N
KKZJGLLVHKMTCM-UHFFFAOYSA-N
KKZJGLLVHKMTCM-UHFFFAOYSA-N

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	ZELUXPWDPVXUEI-ZWKOTPCHSA-N
	QHMBSVQNZZTUGM-ZWKOTPCHSA-N
	QHMBSVQNZZTUGM-ZWKOTPCHSA-N
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	CXOXHMZGEKVPMT-UHFFFAOYSA-N
	NIJJYAXOARWZEE-UHFFFAOYSA-N
	CXOXHMZGEKVPMT-UHFFFAOYSA-N
	YYLPAYRRVSQJRR-KSZLIROESA-N
	VBGLYOIFKLUMQG-UHFFFAOYSA-N
	YCBKSSAWEUDACY-IAGOWNOFSA-N
	YOVRGSHRZRJTLZ-HZPDHXFCSA-N
	YOVRGSHRZRJTLZ-HZPDHXFCSA-N
	VBGLYOIFKLUMQG-UHFFFAOYSA-N
	YCBKSSAWEUDACY-IAGOWNOFSA-N
	VBGLYOIFKLUMQG-UHFFFAOYSA-N
	VBGLYOIFKLUMQG-UHFFFAOYSA-N
	CXOXHMZGEKVPMT-UHFFFAOYSA-N
	CXOXHMZGEKVPMT-UHFFFAOYSA-N
	MYFATKRONKHHQL-UHFFFAOYSA-N
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	CRCWUBLTFGOMDD-UHFFFAOYSA-N
C137DTR5RG	INQSMEFCAIHTJG-UHFFFAOYSA-N
C137DTR5RG	INQSMEFCAIHTJG-UHFFFAOYSA-N
C137DTR5RG	INQSMEFCAIHTJG-UHFFFAOYSA-N
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	LFQSCWFLJHTTHZ-UHFFFAOYSA-N
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	LFQSCWFLJHTTHZ-UHFFFAOYSA-N
	PJVWKTKQMONHTI-HNNXBMFYSA-N
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	PJVWKTKQMONHTI-HNNXBMFYSA-N
144O8QL0L1	DCOPUUMXTXDBNB-UHFFFAOYSA-N
144O8QL0L1	DCOPUUMXTXDBNB-UHFFFAOYSA-N

	PJVWKTKQMONHTI-HNNXBMFYSA-N
144O8QL0L1	DCOPUUMXTXDBNB-UHFFFAOYSA-N
144O8QL0L1	DCOPUUMXTXDBNB-UHFFFAOYSA-N
	PJVWKTKQMONHTI-HNNXBMFYSA-N
	PJVWKTKQMONHTI-HNNXBMFYSA-N
144O8QL0L1	DCOPUUMXTXDBNB-UHFFFAOYSA-N
	PJVWKTKQMONHTI-HNNXBMFYSA-N
	PJVWKTKQMONHTI-HNNXBMFYSA-N
	PJVWKTKQMONHTI-HNNXBMFYSA-N
	PJVWKTKQMONHTI-HNNXBMFYSA-N
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	CRCWUBLTFGOMDD-UHFFFAOYSA-N
	CRCWUBLTFGOMDD-UHFFFAOYSA-N
	CRCWUBLTFGOMDD-UHFFFAOYSA-N
	CRCWUBLTFGOMDD-UHFFFAOYSA-N
	CRCWUBLTFGOMDD-UHFFFAOYSA-N
	CRCWUBLTFGOMDD-UHFFFAOYSA-N
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	KQPKPCNLIDLUMF-UHFFFAOYSA-N
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Birer-Williams et al., "A New Data Repository for Pharmacokinetic Natural Product-Drug Interactions: fr
Drug Metabolism and Disposition

Table S3. Data in the NaPDI Center repository on kratom (Mitragyna speciosa) as of April 2020

dy unique identi	Unique identifier	Natural product binomial	Experiment title	Experiment type name
NPDI-2a2LJw	NPDI-atzv7w	Mitragyna speciosa	Blood brain barrier t	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-_5ld1Q	Mitragyna speciosa	7-Hydroxymitragyni	In Vitro Transporter Inhibitio
NPDI-4xNSSg	NPDI-2HCqSQ	Mitragyna speciosa	Mitraphylline p-gp t	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-2VLnZA	Mitragyna speciosa	Mitragynine P-gp tra	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-iGAFkQ	Mitragyna speciosa	7-Hydroxymitragyni	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-mJ7zbw	Mitragyna speciosa	Inhibition of P-gp by	In Vitro Transporter Inhibitio
NPDI-4xNSSg	NPDI-ruor3g	Mitragyna speciosa	Mitraphylline P-gp t	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-TjrSew	Mitragyna speciosa	7-hyrdoxymitragyni	In Vitro Transporter Kinetics
NPDI-4xNSSg	NPDI-yG9O9A	Mitragyna speciosa	Mitragynine p-gp tra	In Vitro Transporter Kinetics
NPDI-6PgT2w	NPDI-FqB7Jg	Mitragyna speciosa	Kratom Metabolomi	Metabolomics
NPDI-9C7QHg	NPDI-3C6gmg	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-3eovVg	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-4_m2Gw	Mitragyna speciosa	Inhibition of UGT1A	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-4do0FA	Mitragyna speciosa	Inhibition of UGT1A	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-5VhYlA	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-9spGvg	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-bX8XPA	Mitragyna speciosa	No inhibition of UGT	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-ipamgg	Mitragyna speciosa	No inhibition of UGT	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-Nl2Cww	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-NZQ3aw	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-pMOhyQ	Mitragyna speciosa	Inhibition of UGT in	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-Q5Hs5A	Mitragyna speciosa	No inhibition of UGT	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-u96XKg	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-Ve-SYA	Mitragyna speciosa	No inhibition of UGT	In Vitro Enzyme Inhibition
NPDI-9C7QHg	NPDI-ZTY8Qw	Mitragyna speciosa	Inhibition of UGT2B	In Vitro Enzyme Inhibition
NPDI-Algmhw	NPDI-_DqAGQ	Mitragyna speciosa	Control dimethyl sul	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-_MysYg	Mitragyna speciosa	Mitragynine non-inc	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-_rs20g	Mitragyna speciosa	Control dimethyl sul	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI--0S--Q	Mitragyna speciosa	Dimethyl sulfoxide r	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-5_pf-w	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-7sdBtQ	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-dQtQ2g	Mitragyna speciosa	Control dimethyl sul	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-exquAQ	Mitragyna speciosa	Control dimethyl sul	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-J0Eryw	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-LcX0tA	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-LD3MZA	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-sYa6vQ	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-Algmhw	NPDI-Ww9TTQ	Mitragyna speciosa	Mitragynine inducti	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-_xT8iQ	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-1t276A	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-1ZEwLw	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction

NPDI-ct9Vuw	NPDI-20NK8g	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-2go-tA	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-32vFwA	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-3zWYhw	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-5qjXYw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-6g0qjA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-7AsxQw	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-7mTHsg	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-8cNctg	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-8IvpNA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-CeYlQA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-CHz7Cw	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-CUKuJg	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-CyLsKQ	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-d5GHXw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-e6NVBw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-EAC81Q	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-ErfPVw	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-feWibg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-FEZZeA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-GGux5Q	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-HcJ6bw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-iA1bqw	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-iaYQ2g	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-IczeVA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-JfsBYg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-jv2gJw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI--K-VUA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-l9MZKg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-lKNl2g	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-MbgjOA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-Nhyfdg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-PBicLA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-poKS5A	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-PQ_z9Q	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-Q_-B1A	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-Q72VHA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-qToNMQ	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-r08Qaw	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-R0XxIA	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Inductio
NPDI-ct9Vuw	NPDI-R6WiQw	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-SIOBQQ	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-swW6FA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-SzdBUg	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-tQOeEQ	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-tsaRoQ	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-u4e76g	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Inductio

NPDI-ct9Vuw	NPDI-uo42Dw	Mitragyna speciosa	Induction of P-gp ml	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-UwflXA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-v1ALwQ	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-vil20w	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-VRuDCg	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-wkoAog	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI--Wn8sg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-wS5EeQ	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-WzrXMA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-X_71_g	Mitragyna speciosa	POS. CONTROL: Indu	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-x_T2_w	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-XaTzlQ	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-XY34BQ	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-y0jePg	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-yHa9yA	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-Yic2CQ	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-ymobwA	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-YXF4Ww	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-Z3w0mg	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-z5snmg	Mitragyna speciosa	Induction of P-gp ac	In Vitro Transporter Induction
NPDI-ct9Vuw	NPDI-ZI6hHA	Mitragyna speciosa	Induction of CYP1A2	In Vitro Enzyme Induction
NPDI-ct9Vuw	NPDI-ZpaPqg	Mitragyna speciosa	Induction of CYP3A4	In Vitro Enzyme Induction
NPDI-d8OUzg	NPDI-4_UdSg	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-515DHw	Mitragyna speciosa	Inhibition kinetics of	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-71pBaQ	Mitragyna speciosa	Screening of kratom	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-7-Gg-g	Mitragyna speciosa	Screening of kratom	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-A66pwQ	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-bOmVTQ	Mitragyna speciosa	Screening of mitragy	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-EjMg0g	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI--jKvig	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-ksOM2w	Mitragyna speciosa	Inhibition kinetics of	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-o6FZsw	Mitragyna speciosa	Screening of kratom	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-o8WmjA	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-ov597g	Mitragyna speciosa	Screening of mitragy	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-QbMPuw	Mitragyna speciosa	Screening of kratom	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-sfeVpQ	Mitragyna speciosa	Screening of mitragy	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-Tr3Eyg	Mitragyna speciosa	Inhibition kinetics of	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-vr5BAA	Mitragyna speciosa	Screening of mitragy	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-XFPmtA	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-xK3lmw	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-d8OUzg	NPDI-Xrn4xQ	Mitragyna speciosa	IC50 shift determina	In Vitro Enzyme Inhibition
NPDI-dIgOyA	NPDI-38uQKg	Mitragyna speciosa	Mitragynine metabc	In Vitro Enzyme Screen
NPDI-eReNjw	NPDI-_MFsyA	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-0hNq0Q	Mitragyna speciosa	Weak Inhibition of M	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-17YRkg	Mitragyna speciosa	Inhibition of Mitragy	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-1Cjyxg	Mitragyna speciosa	Weak Inhibition of C	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-1vxnrQ	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition

NPDI-eReNjw	NPDI-2seH4Q	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-4AITQg	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-4HfEdA	Mitragyna speciosa	Inhibition of Paynan	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-5LuVNQ	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-7PU97Q	Mitragyna speciosa	Inhibition of Coryna	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-9xzv_Q	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-aGXuxA	Mitragyna speciosa	Weak Inhibition of C	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-aNb3lw	Mitragyna speciosa	Weak Inhibition of P	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-B_7tOA	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-BLzT_g	Mitragyna speciosa	Weak Inhibition of M	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-bXPXRQ	Mitragyna speciosa	Inhibition of Coryna	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-c_gPeA	Mitragyna speciosa	Inhibition of Mitragy	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-cimaKA	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-DLH-JQ	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-eMZPbA	Mitragyna speciosa	Inhibition of 7-hydro	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-gxj_UA	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-iASYyA	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-J2PdQQ	Mitragyna speciosa	Inhibition of Mitragy	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-JqmF7w	Mitragyna speciosa	Inhibition of Speciosc	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-K9DvIg	Mitragyna speciosa	Inhibition of Paynan	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-kew9FQ	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-laH1lA	Mitragyna speciosa	Weak Inhibition of M	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-o56vpA	Mitragyna speciosa	Weak Inhibition of C	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-olaGPQ	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-Oq9KmA	Mitragyna speciosa	Inhibition of Speciog	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-P2Nw6g	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-qMnZyA	Mitragyna speciosa	Weak Inhibition of C	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-QQeDSQ	Mitragyna speciosa	Inhibition of Speciog	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-qWS53g	Mitragyna speciosa	Inhibition of Coryna	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-s8ImuA	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-sN1pZA	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-t32_Ig	Mitragyna speciosa	Control Positive Inhi	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-TTv3Iw	Mitragyna speciosa	Inhibition of Speciosc	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-Ua1CeQ	Mitragyna speciosa	Inhibition of Mitragy	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-U-ajPw	Mitragyna speciosa	Weak Inhibition of 7	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-ULP_qQ	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-V_oQog	Mitragyna speciosa	Weak Inhibition of P	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-WakYGw	Mitragyna speciosa	Inhibition of Paynan	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-WIpfxQ	Mitragyna speciosa	Inhibition of Speicog	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-wo-wRw	Mitragyna speciosa	Inhibition of Paynan	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-XeGihA	Mitragyna speciosa	Weak Inhibition of P	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-XQCOGw	Mitragyna speciosa	Inhibition of Speciosc	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-zKam8g	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-eReNjw	NPDI-Zvn2gg	Mitragyna speciosa	Weak Inhibition of S	In Vitro Enzyme Inhibition
NPDI-FfN_4A	NPDI-d5Gm3Q	Mitragyna speciosa	Mitragynine inhibiti	In Vitro Enzyme Inhibition
NPDI-FfN_4A	NPDI-MpwNXw	Mitragyna speciosa	Mitragynine inhibiti	In Vitro Enzyme Inhibition
NPDI-FfN_4A	NPDI-payj8A	Mitragyna speciosa	Mitragynine inhibiti	In Vitro Enzyme Inhibition

NPDI-FfN_4A	NPDI-TZxzig	Mitragyna speciosa	Mitragynine inhibiti	In Vitro Enzyme Inhibition
NPDI-JHPnhA	NPDI-4k7d3A	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-8GmUTQ	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-cxxGnA	Mitragyna speciosa	Control P-gp digoxin	In Vitro Transporter Kinetics
NPDI-JHPnhA	NPDI-DEOq7g	Mitragyna speciosa	Down regulation of	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-gdI_mg	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-GETspg	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-nWIYpA	Mitragyna speciosa	Down regulation of	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-U0t5zQ	Mitragyna speciosa	Induction of P-gp pr	In Vitro Transporter Inductio
NPDI-JHPnhA	NPDI-Ue8YDg	Mitragyna speciosa	Permeability of mitr	In Vitro Transporter Kinetics
NPDI-JHPnhA	NPDI-WL-VKw	Mitragyna speciosa	Control inhibition of	In Vitro Transporter Inhibitio
NPDI-JHPnhA	NPDI-ye4dPw	Mitragyna speciosa	Down regulation of	In Vitro Transporter Inductio
NPDI-PSB8Vg	NPDI-79TG7g	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-Df2Xyw	Mitragyna speciosa	Negligible inhibition	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-FnVAqw	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-gWxQZg	Mitragyna speciosa	Inhibition of CYP2D6	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-H6ZqbA	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-PSB8Vg	NPDI-jkwBEg	Mitragyna speciosa	Inhibition of CYP2C9	In Vitro Enzyme Inhibition
NPDI-vQCHYg	NPDI-XuAtuQ	Mitragyna speciosa	Characterization of I	Characterization of Material
NPDI-XtvOZQ	NPDI-_PhwAA	Mitragyna speciosa	Inhibition of CYP2D6	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-1tFkCA	Mitragyna speciosa	Inhibition of CYP2C9	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-d0noGQ	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-d-iKog	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-M8nR1A	Mitragyna speciosa	Enzyme kinetics of C	In Vitro Enzyme Kinetics
NPDI-XtvOZQ	NPDI-m-NOOw	Mitragyna speciosa	Enzyme kinetics of C	In Vitro Enzyme Kinetics
NPDI-XtvOZQ	NPDI-o-4ZoA	Mitragyna speciosa	Enzyme kinetics of C	In Vitro Enzyme Kinetics
NPDI-XtvOZQ	NPDI-v2Z25g	Mitragyna speciosa	POS. CONTROL: Inhi	In Vitro Enzyme Inhibition
NPDI-XtvOZQ	NPDI-ypADxQ	Mitragyna speciosa	No inhibition of CYP	In Vitro Enzyme Inhibition
NPDI-Yknaag	NPDI-E56YVg	Mitragyna speciosa	Mitragynine Inhibiti	In Vitro Transporter Inhibitio
NPDI-Yknaag	NPDI-vs2diA	Mitragyna speciosa	R123 Transport Subs	In Vitro Transporter Kinetics

om Chemical Characterization to Clinical Studies",

Overall effect

In Vitro Transport
In Vitro Transporter Inhibition
In Vitro Transport
No In Vitro Transport Activity
No In Vitro Transport Activity
In Vitro Transporter Inhibition
In Vitro Transport
No In Vitro Transport Activity
No In Vitro Transport Activity

In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
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In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Transporter Induction
In Vitro Enzyme Induction
In Vitro Enzyme Non-induction

In Vitro Enzyme Induction
In Vitro Transporter Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Transporter Induction
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In Vitro Transporter Induction
In Vitro Transporter Induction
In Vitro Transporter Induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Transporter Induction
In Vitro Transporter Induction
In Vitro Enzyme Induction
In Vitro Enzyme Non-induction
In Vitro Enzyme Non-induction
In Vitro Transporter Induction
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In Vitro Enzyme Induction
In Vitro Transporter Induction

In Vitro Transporter Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Non-induction
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In Vitro Transporter Induction
In Vitro Transporter Induction
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In Vitro Transporter Induction
In Vitro Enzyme Induction
In Vitro Enzyme Induction
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
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In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Detectable Metabolism
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition

In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
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In Vitro Enzyme Negligible Inhibition
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In Vitro Enzyme Negligible Inhibition
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In Vitro Enzyme Negligible Inhibition
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In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition

In Vitro Enzyme Inhibition
In Vitro Transporter Induction
In Vitro Transporter Induction
In Vitro Transport
In Vitro Transporter Down Regulation
In Vitro Transporter Induction
In Vitro Transporter Induction
In Vitro Transporter Down Regulation
In Vitro Transporter Induction
No In Vitro Transport Activity
In Vitro Transporter Inhibition
In Vitro Transporter Down Regulation
In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition

In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Enzyme Inhibition
In Vitro Detectable Kinetic Metabolism
In Vitro Detectable Kinetic Metabolism
In Vitro Detectable Kinetic Metabolism
In Vitro Enzyme Inhibition
In Vitro Enzyme Negligible Inhibition
In Vitro Transporter Inhibition
In Vitro Transport

Object compound name	Object metabolite compound name
mitragynine	
calcein-am	
mitraphylline	
mitragynine	
7-hydroxymitragynine	
calcein-am	
mitraphylline	
7-hydroxymitragynine	
mitragynine	
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide
4-methylumbelliferone	4-methylumbelliferone glucuronide

midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
diclofenac	4'-hydroxydiclofenac
midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
diclofenac	4'-hydroxydiclofenac
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
dextromethorphan	dextrorphan
dextromethorphan	dextrorphan
midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
midazolam	1'-hydroxymidazolam
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
diclofenac	4'-hydroxydiclofenac
diclofenac	4'-hydroxydiclofenac
mitragynine	7-hydroxymitragynine
phenacetin	acetaminophen
diclofenac	4'-hydroxydiclofenac
dextromethorphan	dextrorphan
phenacetin	acetaminophen
phenacetin	acetaminophen

testosterone	6beta-hydroxytestosterone
dextromethorphan	dextrorphan
diclofenac	4'-hydroxydiclofenac
phenacetin	acetaminophen
midazolam	1'-hydroxymidazolam
testosterone	6beta-hydroxytestosterone
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
testosterone	6beta-hydroxytestosterone
amodiaquine	n-desethylamodiaquine
testosterone	6beta-hydroxytestosterone
diclofenac	4'-hydroxydiclofenac
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
diclofenac	4'-hydroxydiclofenac
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
testosterone	6beta-hydroxytestosterone
amodiaquine	n-desethylamodiaquine
amodiaquine	n-desethylamodiaquine
dextromethorphan	dextrorphan
midazolam	1'-hydroxymidazolam
phenacetin	acetaminophen
amodiaquine	n-desethylamodiaquine
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
testosterone	6beta-hydroxytestosterone
testosterone	6beta-hydroxytestosterone
midazolam	1'-hydroxymidazolam
dextromethorphan	dextrorphan
amodiaquine	n-desethylamodiaquine
diclofenac	4'-hydroxydiclofenac
diclofenac	4'-hydroxydiclofenac
midazolam	1'-hydroxymidazolam
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
amodiaquine	n-desethylamodiaquine
dextromethorphan	dextrorphan
phenacetin	acetaminophen
midazolam	1'-hydroxymidazolam
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
amodiaquine	n-desethylamodiaquine
mephenytoin, (s)-	4-hydroxymephenytoin, (s)-
phenacetin	acetaminophen
diclofenac	4'-hydroxydiclofenac
3-cyano-7-ethoxycoumarin	3-cyano-7-hydroxycoumarin
3-cyano-7-ethoxycoumarin	3-cyano-7-hydroxycoumarin
3-[2-(n,n-diethyl-n-methylammoni	3-[2-(n,n-diethyl-n-methylammonium)ethyl]-

7-benzyloxy-4-(trifluoromethyl)-co 7-hydroxy-4-(trifluromethyl)-coumarin

digoxin

mitragynine
digoxin

luciferin 6â€™benzyl ether (luciferi luciferin
luciferin 6â€™benzyl ether (luciferi luciferin
ethylene glycol ester of luciferin 6â luciferin
ethylene glycol ester of luciferin 6â luciferin
6â€™deoxyluciferin (luciferin h) luciferin
6â€™deoxyluciferin (luciferin h) luciferin

ethylene glycol ester of luciferin 6â luciferin
6â€™deoxyluciferin (luciferin h) luciferin
ethylene glycol ester of luciferin 6â luciferin
luciferin 6â€™benzyl ether (luciferi luciferin
luciferin 6â€™benzyl ether (luciferi luciferin
6â€™deoxyluciferin (luciferin h) luciferin
ethylene glycol ester of luciferin 6â luciferin
6â€™deoxyluciferin (luciferin h) luciferin
luciferin 6â€™benzyl ether (luciferi luciferin
rhodamine 123
rhodamine 123

Precipitant compound name

7-hydroxymitragynine

mitragynine

7-hydroxymitragynine
buprenorphine
diclofenac
7-hydroxymitragynine
mitragynine
mitragynine
ketamine
ketamine
mitragynine
diclofenac
buprenorphine
7-hydroxymitragynine
diclofenac
ketamine
buprenorphine
dimethyl sulfoxide
mitragynine
dimethyl sulfoxide
dimethyl sulfoxide
mitragynine
mitragynine
dimethyl sulfoxide
dimethyl sulfoxide
mitragynine
mitragynine
mitragynine
mitragynine
mitragynine
mitragynine
speciogynine
isorotundifoline
mitragynine

rifampicin
mitragyna speciosa alkaloid rich fraction
omeprazole
rifampicin
paynantheine
7-hydroxymitragynine
corynoxine b
mitragynine
speciogynine
mitragyna speciosa alkaloid rich fraction
isospeciofoline
corynoxine
7betaâ€hydroxyâ€7hâ€mitraciliatine
methanolic extract of kratom
7-hydroxymitragynine
corynoxine
speciogynine
speciogynine
7-hydroxymitragynine
isorotundifoline
corynoxine
mitragyna speciosa alkaloid rich fraction
dexamethasone
omeprazole
paynantheine
paynantheine
isospeciofoline
corynoxine b
corynoxine
methanolic extract of kratom
methanolic extract of kratom
corynoxine b
7betaâ€hydroxyâ€7hâ€mitraciliatine
paynantheine
7betaâ€hydroxyâ€7hâ€mitraciliatine
methanolic extract of kratom
mitragynine
corynoxine b
paynantheine
corynoxine
corynoxine
speciogynine
mitragyna speciosa alkaloid rich fraction
mitragyna speciosa alkaloid rich fraction
corynoxine b
isospeciofoline
7betaâ€hydroxyâ€7hâ€mitraciliatine

isorotundifoline
mitragyna speciosa alkaloid rich fraction
isospeciofoline
mitragynine
7-hydroxymitragynine
isorotundifoline
isospeciofoline
7-hydroxymitragynine
7-hydroxymitragynine
dexamethasone
isospeciofoline
mitragynine
7betaâ€hydroxyâ€7hâ€mitraciliatine
mitragynine
7betaâ€hydroxyâ€7hâ€mitraciliatine
isorotundifoline
isorotundifoline
corynoxine b
methanolic extract of kratom
paynantheine
speciogynine
methanolic extract of kratom
mitragynine
mitragynine
methanolic extract of kratom
methanolic extract of kratom
mitragynine
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mitragynine
mitragynine
mitragynine

speciogynine
mitragynine
mitragynine
corynantheidine
7-hydroxymitragynine

speciociliatine
quinidine
paynantheine
alpha-naphthoflavone
corynantheidine
ketoconazole
corynantheidine
paynantheine
speciogynine
mitragynine
corynantheidine
mitragynine
7-hydroxymitragynine
7-hydroxymitragynine
7-hydroxymitragynine
(s)-(+)-n-3-benzylnirvanol
7-hydroxymitragynine
mitragynine
speciociliatine
paynantheine
ketoconazole
mitragynine
corynantheidine
7-hydroxymitragynine
speciogynine
speciogynine
corynantheidine
speciogynine
corynantheidine
montelukast
speciogynine
sulfaphenazole
speciociliatine
mitragynine
7-hydroxymitragynine
speciociliatine
paynantheine
paynantheine
speciogynine
paynantheine
paynantheine
speciociliatine
speciociliatine
speciociliatine
mitragynine
mitragynine
mitragynine

mitragynine
rifampicin
rifampicin

mitragynine
rifampicin
rifampicin
mitragynine
rifampicin

quinidine
quinidine
ketoconazole
methanolic extract of kratom
quinidine
methanolic extract of kratom
sulfaphenazole
methanolic extract of kratom

mitragynine
mitragynine
quinidine
ketoconazole

sulfaphenazole
mitragynine
mitragynine

Enzyme name

UGT2B7
UGT1A1
UGT1A1
UGT1A1
UGT1A1
UGT2B7
UGT2B7
UGT
UGT
UGT2B7
UGT
UGT
UGT
UGT1A1
UGT2B7
CYP1A2
CYP2D6
CYP3A4
CYP2D6
CYP3A4
CYP1A2
CYP3A4
CYP1A2
CYP1A2
CYP3A4
CYP1A2
CYP3A4
CYP2D6

CYP1A2
CYP3A4

CYP3A4

CYP1A2
CYP3A4

CYP3A4
CYP3A4

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CYP1A2

CYP1A2
CYP3A4
CYP3A4

CYP1A2
CYP3A4
CYP3A
CYP3A
CYP2C9
CYP3A
CYP3A
CYP2C9
CYP3A
CYP2D6
CYP2D6
CYP2D6
CYP3A
CYP3A
CYP3A
CYP2D6
CYP3A
CYP3A
CYP2D6
CYP2C9
CYP2C9
CYP3A4
CYP1A2
CYP2C9
CYP2D6
CYP1A2
CYP1A2

CYP3A5
CYP2D6
CYP2C9
CYP1A2
CYP3A5
CYP3A5
CYP2C19
CYP3A5
CYP2C8
CYP3A5
CYP2C9
CYP3A5
CYP2D6
CYP2C9
CYP2C19
CYP2C19
CYP3A5
CYP2C8
CYP2C8
CYP2D6
CYP3A5
CYP1A2
CYP2C8
CYP3A5
CYP2D6
CYP3A5
CYP3A5
CYP3A5
CYP2D6
CYP2C8
CYP2C9
CYP2C9
CYP3A5
CYP2C19
CYP2C8
CYP2D6
CYP1A2
CYP3A5
CYP2C19
CYP2C19
CYP2C8
CYP2C19
CYP1A2
CYP2C9
CYP2C19
CYP1A2
CYP2D6

CYP3A4

CYP3A4
CYP3A4
CYP2D6
CYP2D6
CYP2C9
CYP2C9

CYP2D6
CYP2C9
CYP2D6
CYP3A4
CYP3A4
CYP2C9
CYP2D6
CYP2C9
CYP3A4

Transporter name	Control data	Test system name	IC50 shift data
P-gp (ABCB1)	FALSE	Other cells	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
P-gp (ABCB1)	FALSE	MDCK transfected ce	FALSE
	FALSE		FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	FALSE	Baculovirus-insect ce	FALSE
	TRUE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	TRUE	HepG2 cell line	FALSE
	TRUE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	TRUE	HepG2 cell line	FALSE
	TRUE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE

	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
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	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE

P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
P-gp (ABCB1)	FALSE	HepG2 transfected c	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	HepG2 cell line	FALSE
	FALSE	Pooled human liver r	TRUE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human intest	TRUE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	TRUE
	FALSE	Pooled human liver r	TRUE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human intest	TRUE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human intest	FALSE
	FALSE	Pooled human liver r	FALSE
	FALSE	Pooled human intest	FALSE
	FALSE	Pooled human intest	FALSE
	FALSE	Pooled human liver r	TRUE
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P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
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P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE
P-gp (ABCB1)	FALSE	Caco-2 cells	FALSE

Research organization's overall effect cutof	ditional informat
$P < 0.001$	
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positive control verapamil (22.3Â± 1.4 Î¼M)	
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ER of 2	
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IC50<10 µM for reversible inhibition and IC50s	
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50% inhibition at the highest tested concer	Three methanoli
IC50<10 µM for reversible inhibition and IC50s	
50% inhibition at the highest tested concentration	
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IC50<10 µM for reversible inhibition and IC50s	
N/A	
50% inhibition at the highest tested concer	Three methanoli
IC50<10 µM for reversible inhibition and IC50s	
50% inhibition at the highest tested concentration	
50% inhibition at the highest tested concer	Three methanoli
50% inhibition at the highest tested concentration	
N/A	
50% inhibition at the highest tested concentration	
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IC50<10 µM for reversible inhibition and IC50s	

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(not provided)	
(not provided)	
p < 0.05 compared with control	
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	Comparison with
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High probability of interaction if their IC50	values are less th
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High probability of interaction if their IC50	Positive control
High probability of interaction if their IC50	Positive control
High probability of interaction if their IC50	values are less th
Unspecified	p<0.05 Values de
Unspecified	Positive control -

Experimental conditions comment

The amount of protein, the incubation time and the concentration of 4-MU used in the measurement of 4-MU glu
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Pooled human liver microsomes were purchased from Sigma-Aldrich; The enzyme activity assay mixture (250 Î¼L)
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ɔntrol: 50 uM omeprazole, ~4 ± 2 x 1012 copies

ɔntrols and results: CYP1A2: 50 uM omeprazole, mean ~1.2 ± 0.2-fold, n = 2 CYP2D6: 5uM quinidine,
e control used
ɔression of CYP3A4 was only slightly induced by mitragynine at all concentrations tested. Although this induction w

5 uM dexamethasone with ~1.6 ± 0.4 x 1013 copies

icle control used; unknown what solvent(s) and what % of those solvent(s) constituted the vehicle control.
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7â€benzyloxyâ€4â€(trifluoromethyl)coumarin (BFC) 2Î¼M was the fluorescent substrate used for CYP3A4 activity r

Positive control
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3â€Cyanoâ€7â€ethoxycoumarin (CEC) 1 Î¼M was the fluorescent substrate used for CYP1A2 activity measurement
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A cocktail of probe substrates for CYP2C9 (diclofenac), CYP2D6 (dextromethorphan), and CYP3A (midazolam) was u
Methanol (0.8 % v/v) served as solvent control. 6',7'-Dihydroxybergamottin (1 and 2 ÂµM) served as a positive con
Methanol (0.8 % v/v) served as solvent control. Sulphaphenazole (1 ÂµM), quinidine (2 ÂµM), and ketoconazole (0
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Methanol (0.8 % v/v) served as solvent control. Quinidine (2 ÂµM) served as positive control inhibitors of CYP2D6 a
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Table S2

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Table S2

Positive controls sulfaphenazole, quinidine, and ketoconazole were purchased from Sigma Chemicals (St. Louis, US
M. speciosa methanolic extract was prepared in-house from the leaves of the plant. This assay was carried out usir
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ı Literature:A recent report [1] found that depending on source material, mitragyninewas detected in kratom (M. sp
Mitragynine was isolated in-house. This assay was carried out using the P450-Gloâ„¢ Screening Systems from Prom
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Positive inhibitors which are sulfaphenazole, quinidine and ketoconazole were purchased from Sigma Chemicals (S
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Mitragynine was isolated in-house. This assay was carried out using the P450-Gloâ„¢ Screening Systems from Prom
Preincubated with KRB for 60 min
· verapamil (5 µM) ER of 7.4

Experimental results comment

positive control verapamil (22.3Â± 1.4 Î¼M)Fig 1S (with exact values in text pg 574)
p<0.001ER for 10 uM was 5.9 also significant(Table 4)
Results above for 5 uMER for 10 uM values reported: 1.1 N=3(Table 3)
ER for 10 uM also 1.2(Table 4)
positive control verapamil (22.3Â± 1.4 Î¼M) Fig 1S (with exact values in text pg 574)
ER for 10 uM is 3.4p<0.001(Table 3)
ER for 10 uM also 1.2(Table 3)
ER for 10 uM also 1.1(Table 4)

Concentration ofÂ precipitant and % inhibition of UGT2B7 (values estimated from figure 5)0.01 Î¼M: 3 Â± 5%0.1 Î¼
The IC50 values were all greater than the highest concentrations used (IC50 > 1000 Î¼M) since inhibition at more t
Concentration ofÂ precipitant and % inhibition of UGT1A1 (values estimated from figure 4) (p < 0.05 for all values)
Concentration ofÂ precipitant and % inhibition of UGT1A1 (values estimated from figure 4)0.01 Î¼M: 6 Â± 1%0.1 Î¼
The IC50 values were all greater than the highest concentrations used (IC50 > 100 Î¼M) since inhibition at more th
The IC50 values were all greater than the highest concentrations used (IC50 > 100 Î¼M) since inhibition at more th
Concentration ofÂ precipitant and % inhibition of UGT2B7 (values estimated from figure 5)0.01 Î¼M: -5 Â± 6%0.1 Î
The IC50 values were all greater than the highest concentrations used (IC50 > 1000 Î¼M) since inhibition at more tl
The IC50 values were all greater than the highest concentrations used (IC50 > 100 Î¼M) since inhibition at more tha
Concentration ofÂ precipitant and % inhibition of UGT2B7 (values estimated from figure 5)0.01 Î¼M: -1 Â± 3%0.1 Î
Concentration of precipitant and % inhibition of pooled human liver microsomes (values estimated from figure 3) (
The IC50 values were all greater than the highest concentrations used (IC50 > 100 Î¼M) since inhibition at more tha
Concentration of precipitant and % inhibition of pooled human liver microsomes (values estimated from figure 3) (
The IC50 values were all greater than the highest concentrations used (IC50 > 1000 Î¼M) since inhibition at more t
Concentration ofÂ precipitant and % inhibition of UGT2B7 (values estimated from figure 5)0.01 Î¼M: -8 Â± 4%0.1 Î
Figure 2. 3 copies, 0 copy number. Positive control: 50 uM omeprazole, ~4-6 x 1012 copies
"There was no significant change in the mRNA expression of CYP2D6 when the HepG2 cells were treated with mitr
Figure 3. P-value not reported.Â Positive controls and results: CYP1A2: 50 uM omeprazole, mean ~1.2Â Â± 0.2-fold
Fig. 2. Approximately ~1.2-1.5 x 1012 copies. No positive control used.
(Figure 2)The expression of CYP3A4 was only slightly induced by mitragynine at all concentrations tested. Although
68.5% of induction compared to positive control at [25 uM]
Figure 2. Approximately 4.9 Â± 0.3 x 1012 copies. Positive control: 5 uM dexamethasone with ~1.6Â Â± 0.4 x 1013
(Figure 4)
"The induction was only statistically significant at 25 lM and induction relative to omeprazole was approximately 4
"Mitragynine appeared to moderately induce the enzymatic activity of CYP3A4. The increase was gradual and the c
the protein expression of CYP1A2 showed an increased in relative values from 0.5uM onwards as compared to con
The protein expression of CYP3A4 was slightly induced after treatment with mitragynine, with higher relative prot
CYP2D6 protein expression was found to be increased within the range of 1-5 uM of mitragynine relative to the ur
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.57 Â± 0.03 fold (p < 0.01)1.1 Î¼M: 1.07
Estimated from Figure 3a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 6.2 Â± 0.4 fold (p < 0.01)1.1 Î¼M: 3.3 Â± 0.2
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.95 Â± 0.1 fold 1.1 Î¼M: 0.9 Â± 0.05 fold

Positive controlEstimated from Figure 2a***P<0.001
Estimated from Figure 4bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 0.45 Â± 0.06 fold (p < 0.01)3.3 Î¼g/m
Positive control***P<0.001
Positive controlEstimated from Figure 2b***P<0.001
Estimated from Figure 4aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.3 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.2 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 2.0 Â± (
Estimated from Figure 2b***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 1.8 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.1 Â± 0.(
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.1 fold (p <0.01)1.1 Î¼M: 1.3 Â± 0.1
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.1 fold (p < 0.01)1.1 Î¼M: 1.5 Â± 0.1
Estimated from Figure 2bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.0 Â± 0.05 fold (p < 0.05)3.3 Î¼g/ml
Estimated from Figure 3a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 3.4 Â± 0.3 fold (p < 0.05)1.1 Î¼M: 2.1 Â± 0.2
Estimated from Figure 2b***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 1.9 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.0 Â± 0.(
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.9 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.6 Â± (
Estimated from Figure 4a***P<0.001 for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.2 Â± 0.1 fold (p < 0.01)3.3 Î¼g/ml: 1.4
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.3 Â± 0.1 fold (p < 0.01)1.1 Î¼M: 1.7 Â± 0.1
Estimated from Figure 4aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.2 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.7 Â±0
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.2 Â± 0.1 fold1.1 Î¼M: 1.0 Â± 0.05 fold
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.05 Â± 0.1 fold 1.1 Î¼M: 1.0 Â± 0.05 fold
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.05 fold (p < 0.01)1.1 Î¼M: 1.3 Â±
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.9 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.3 Â± (
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.8 Â± 0.4 fold (p < 0.05)1.1 Î¼M: 2.7 Â± (
Estimated from Figure 4a***P<0.001 for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.7 Â± 0.3 fold (p < 0.001)3.3 Î¼g/ml: 1
Positive controlEstimated from Figure 4a*** P<0.001
Positive controlEstimated from Figure 3b***P<0.001
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.0 Â± 0.05 fold 1.1 Î¼M: 0.9 Â± 0.1 fold
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.85 Â± 0.05 fold1.1 Î¼M: 0.80 Â± 0.05 fo
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.6 Â± 0.1
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.8 Â± 0.3 fold (p < 0.05)1.1 Î¼M: 2.3 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.9 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.1 Â± (
Estimated from Figure 3a***P<0.001 for 30Â Î¼g/ml (see above)10 Î¼g/ml: 3.4 Â± 0.4 fold (p < 0.05)3.3 Î¼g/ml: 1.6
Estimated from Figure 2aMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 1.9 Â± 0.1 fold (p < 0.05)3.3 Î¼g/ml:
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.9 Â± (
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.3 Â± 0.4 fold (p < 0.05)1.1 Î¼M: 1.5 Â± (
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.8 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.9 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.1 Â± (
Estimated from Figure 3bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.5 Â± 0.3 fold (p < 0.05)3.3 Î¼g/ml:
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.6 Â± 0.3 fold (p < 0.01)1.1 Î¼M: 1.8 Â± (
Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.7 Â± 0.2
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.7 Â± 0.4 fold (p < 0.05)1.1 Î¼M: 1.8 Â± (
Estimated from Figure 4b*** p < 0.001 for 10Â Î¼M (see above)3.3 Î¼M: 0.51 Â± 0.04 fold (p < 0.05)1.1 Î¼M: 1.01 A
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.5 Â± 0.5 fold (p < 0.01)1.1 Î¼M: 1.0 Â± (
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.5 Â± 0.3 fold (p < 0.01)1.1 Î¼M: 1.5 Â± (
Estimated from Figure 3a***P<0.001 for 30Â Î¼g/ml (see above)10 Î¼g/ml: 4.4 Â± 0.9 fold (p < 0.01)3.3 Î¼g/ml: 1.9
Estimated from Figure 3bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 3.6 Â± 0.5 fold (p < 0.01)3.3 Î¼g/ml:
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.2 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.0 Â± (
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.1 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.3 Â± (
Estimated from Figure 4aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.6 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.2 Â± (

Estimated from Figure 4a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.4 Â± 0.0
Estimated from Figure 2aMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.0 Â± 0.3 fold (p < 0.05)3.3 Î¼g/ml:
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.9 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.4 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.3 Â± 0.3 fold1.1 Î¼M: 0.9 Â± 0.1 fold
Estimated from Figure 3bMeasurement forÂ 10Â Î¼M (see above)3.3 Î¼M: 2.2 Â± 0.2 fold (p < 0.05)1.1 Î¼M: 1.7 Â±
Estimated from Figure 3bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.1 fold (p < 0.05)1.1 Î¼M: 1.1 Â± (
Estimated from Figure 2aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 2.0 Â± 0.3 fold (p < 0.05)1.1 Î¼M: 1.2 Â± (
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.47 Â± 0.06 fold (p < 0.01)1.1 Î¼M: 1.06
Estimated from Figure 3a***P<0.001 for 10Â Î¼M (see above)3.3 Î¼M: 5.2 Â± 0.7 fold (p < 0.01)1.1 Î¼M: 3.8 Â± 0.7
Positive controlEstimated from Figure 4b*** P<0.001
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.57 Â± 0.04 fold (p < 0.05)1.1 Î¼M: 1.02
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.60 Â± 0.05 fold (p < 0.05)1.1 Î¼M: 1.00
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.53 Â± 0.07 fold (p < 0.01)1.1 Î¼M: 0.97
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.2 Â± 0.5 fold (p < 0.01)1.1 Î¼M: 2.3 Â± (
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.6 Â± 0.25 fold (p < 0.05)1.1 Î¼M: 1.0 Â±
Estimated from Figure 2bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 1.3 Â± 0.2 fold1.1 Î¼M: 1.0Â± 0.05 fold
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.55 Â± 0.06 fold (p < 0.05)1.1 Î¼M: 1.03
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.58 Â± 0.03 fold (p < 0.05)1.1 Î¼M: 0.97
Estimated from Figure 4bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 0.50 Â± 0.02 fold (p < 0.01)3.3 Î¼g/m
Estimated from Figure 4bMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 0.57 Â± 0.08 fold (p < 0.05)1.1 Î¼M: 1.05
Estimated from Figure 3aMeasurement for 10Â Î¼M (see above)3.3 Î¼M: 3.7 Â± 0.6 fold (p < 0.01)1.1 Î¼M: 2.2 Â±0
Estimated from Figure 2bMeasurement for 30Â Î¼g/ml (see above)10 Î¼g/ml: 2.0 Â± 0.05 fold (p < 0.05)3.3 Î¼g/ml
A 7-fold shift in IC50was observed towards CYP3A activity in HLM, 18.9 Â±1.8 vs. 2.6 Â±0.3 ÂµM, in absence and pr
The KIand kinactvalues for mitragynine towards CYP3A activity in HLM were 4.1 Â±Â 0.7 ÂµM and 0.051 Â± 0.002 r
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
A 7-fold shift in IC50was observed towards CYP3A activity in HIM, 21.9 Â±2.7 vs. 3.2 Â±0.3 ÂµM, in absence and pr
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
A 7-fold shift in IC50was observed towards CYP3A activity in HLM, 18.9 Â±1.8 vs. 2.6 Â±0.3 ÂµM, in presence and a
ısed for the IC50shift determination.Methanol (0.8 % v/v) served as solvent control. Tienilic acid (0.4 and 0.8 ÂµM),
Mitragynine was shown to be a strong competitive inhibitor of CYP2D6 activity, with a Kiof 0.97 Â±Â 0.07 ÂµM, 1.2
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP activity in HLM. Mitragynine a
A 7-fold shift in IC50was observed towards CYP3A activity in HIM, 21.9 Â±2.7 vs. 3.2 Â±0.3 ÂµM, in presence and al
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The KIand kinactvalues for mitragynine towards CYP3A activity in HIM were 4.5 Â±Â 1.1 ÂµM and 0.072 Â± 0.006 m
Mitragynine and kratom extracts showed concentration-dependent inhibition of CYP3A activity in HIM. Mitragynin
ısed for the IC50shift determination.Methanol (0.8 % v/v) served as solvent control. Tienilic acid (0.4 and 0.8 ÂµM),
ısed for the IC50shift determination.Methanol (0.8 % v/v) served as solvent control. Tienilic acid (0.4 and 0.8 ÂµM),
ısed for the IC50shift determination.Methanol (0.8 % v/v) served as solvent control. Tienilic acid (0.4 and 0.8 ÂµM),
% remaining was inferred from panel A of Fig 5 where the total contribution of each enzyme to MTG metabolism is
% result estimated from Figure S2 at around 30 ÂµM
% result estimated from Figure 2 at around 30 ÂµM
% result estimated from Figure 2 at around 100 ÂµM
% result estimated from Figure 3 at around 100 ÂµM
% result estimated from Figure S4 at around 100 ÂµM

% result estimated from Figure S3 at around 100 ÂµM

% result estimated from Figure S5 at around 100 ÂµM

% result estimated from Figure 3 at around 100 ÂµM

% result estimated from Figure 3 at around 30 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
% result estimated from Figure 2 at around 100 ÂµM
% result estimated from Figure 3 at around 100 ÂµM
% result estimated from Figure 2 at around 100 ÂµM
% result estimated from Figure S4 at around 100 ÂµM
% result estimated from Figure S4 at around 100 ÂµM
% result estimated from Figure S4 at around 100 ÂµM

% result estimated from Figure S4 at around 100 ÂµM
% result estimated from Figure 2 at around 100 ÂµM
% result estimated from Figure S3 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM

% result estimated from Figure 2 at around 30 ÂµM
% result estimated from Figure 3 at around 30 ÂµM
% result estimated from Figure S4 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
% result estimated from Figure 3 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
% result estimated from Figure 3 at around 100 ÂµM

% result estimated from Figure S2 at around 30 ÂµM

% result estimated from Figure S3 at around 100 ÂµM
% result estimated from Figure 2
% result estimated from Figure S4 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
% result estimated from Figure S2 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
% result estimated from Figure S5 at around 100 ÂµM
% result estimated from Figure S3 at around 100 ÂµM
% result estimated from Figure S3 at around 30 ÂµM
% result estimated from Figure S3
IC50 was not determined because inhibition was < 50%.Tranylcypromine was used as a positive control.(Table 2, Fi
Furafylline is used as the positive control(Table 2, Figure 2)
Quinidine was used as the positive control(Table 2, Figure 2)

Ketoconazole was used as the positive control.(Table 2, Figure 2)

Mean taken from text. SD estimated from Figure 3a.

Estimate from Fig 3a

Figure 2a for Papp ratio

% Inhibition mean taken from text. SD estimated from Figure 3b.
Positive control
% enzyme inhibition versus precipitant concentration:Values estimated from Figure 1d. In some cases, SEM could r
Positive control
% enzyme inhibition versus precipitant concentration:Values estimated from Figure 1d. In some cases, SEM could r
Positive control
IC50 not determined due to the less than 50% of inhibition.% enzyme inhibition versus precipitant concentration:V
peciosa) products at a concentration range between 1 and 6% of leaf content (10 to 60 mg/g) and that 7-hydroxymi
IC50 values from Table 1, Ki values from Table 3% enzyme inhibition versus precipitant concentration:Values estim
IC50 values from Table 1, Ki values from Table 3% enzyme inhibition versus precipitant concentration:Values estim
Positive controlIC50 values from Table 1% enzyme inhibition versus precipitant concentration:Values estimated frc
Positive controlIC50 values from Table 1% enzyme inhibition versus precipitant concentration:Values estimated frc
Km and Vmax from Table 2
Km and Vmax from Table 2
Km and Vmax from Table 2
Positive controlIC50 values from Table 1% enzyme inhibition versus precipitant concentration:Values estimated frc
IC50 values from Table 1, Ki values from Table 3% enzyme inhibition versus precipitant concentration:Values estim
Results for Mitragynine+R123 were statistically significant ($p<0.05$) vs R123 alone. Values from Fig. 5
Values from Fig 5

Internal: Additional comments

Experimental conditions tab:Â Uchaipichat et al can be found here http://dmd.aspetjournals.org/content/dmd/32

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han 50% did not occur at the highest concentration.Concentration of precipitant and % inhibition of pooled human

an 50% did not occur at the highest concentration.Concentration ofÂ precipitant and % inhibition of pooled human

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p<0.05 for all values)0.01 Î¼M: 27 Â± 2%0.1 Î¼M: 39 Â± 1% 1 Î¼M: 43 Â± 3% 10 Î¼M: 55 Â± 1% 100 Î¼M: 61 Â± 2%

an 50% did not occur at the highest concentration.Concentration ofÂ precipitant and % inhibition of pooled human

p<0.05 for all values)0.01 Î¼M: 8 Â± 3%0.1 Î¼M: 9 Â± 2% 1 Î¼M: 20 Â± 1% 10 Î¼M: 21 Â± 1% 100 Î¼M: 41 Â± 1%10

Experimental conditions tab:Â Uchaipichat et al can be found here http://dmd.aspetjournals.org/content/dmd/32

Experimental conditions tab:Â Uchaipichat et al can be found here http://dmd.aspetjournals.org/content/dmd/32

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, n = 2 CYP2D6: 5uM quinidine, mean ~1.2Â Â± 0.1 fold, n = 2 CYP3A4: 5uM dexamethasone, mean ~1.2Â Â± 0.1 fo

this induction was statistically significant within the range of 1-5 uM of mitragynine, the induction relative to dexa

Mitragynine appeared to induce the mRNA expression of CYP1A2 in a concentration-dependent manner; significar

copies

0.7% (Fig. 4a)."

changes in the enzymatic activity were minimal. The greatest increase in CYP3A4 enzymatic activity, approximately

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ein expression at concentrations of 0.1uM and above, with the highest induction occurring at 0.5 uM relative to un

ntreated control. [...] Although the corresponding mRNA expression of CYP2D6 did show slight increase in the mRN

Â± 0.03 fold

fold (p < 0.05)

ıl: 0.95 Â± 0.06 fold

0.05 fold
0.1 fold (p < 0.05)
)5 fold
fold
l fold
: 1.1 Â± 0.05 fold
2 fold
)5 fold
0.05 fold
1 Â±0.2 fold
l fold
).2 fold

ł
ŧ 0.1 fold
0.1 fold
0.6 fold (p < 0.05)
.5 Â± 0.1 fold

ɔld
l fold
0.4 fold (p < 0.05)
0.05 fold
5 Â± 0.2 fold
1.2 Â± 0.1 fold
0.1 fold
0.2 fold
0.1 fold
0.05 fold
1.2 Â± 0.05 fold
0.2 fold
2 fold
0.2 fold
Â± 0.04 fold
0.1 fold
0.1 fold
9 Â± 0.2 fold
2.1 Â± 0.1 fold (p < 0.05)
0.1 fold
0.1 fold
0.1 fold

)5 fold
1.2 Â± 0.05 fold
0.1 fold

± 0.2 fold
0.1 fold
0.05 fold
 Â± 0.05 fold
 fold (p < 0.05)

 Â± 0.06 fold
 Â± 0.10 fold
 Â± 0.07 fold
0.5 fold (p < 0.05)
± 0.05 fold

 Â± 0.03 fold
 Â± 0.08 fold
ıl: 1.03 Â± 0.07 fold
 Â± 0.04 fold
).1 fold (p < 0.05)
: 1.1 Â± 0.05 fold
esenceÂ of NADPH, respectively. [IC50values (Mean Â± SEM) were determined using nonlinear least-squares regre
nin-1, 4.0 Â±Â 0.5 ÂµM and 0.057 Â± 0.002 min-1, and 5.9 Â±Â 0.9 ÂµM and 0.17 Â± 0.01 min-1, respectively, for t
at 10 ÂµM inhibited CYP2C9, CYP2D6, and CYP3A activity by 42%, 87%, and 50%, respectively. Kratom extracts at 2
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, paroxetine (0.25 and 0.5 ÂµM), and 6',7'-dihydroxybergamottin (1 and 2 ÂµM) served as positive control inhibitor
!5 Â±Â 0.09 ÂµM, and 0.95 Â± 0.11 ÂµM, respectively, for three individual experiments. [Ki(Mean Â± SEM) values w
at 10 ÂµM inhibited CYP2C9, CYP2D6, and CYP3A activity by 42%, 87%, and 50%, respectively. Kratom extracts at 2
bsence ofÂ NADPH, respectively. [IC50values (Mean Â± SEM) were determined using nonlinear least-squares regre
at 10 ÂµM inhibited CYP2C9, CYP2D6, and CYP3A activity by 42%, 87%, and 50%, respectively. Kratom extracts at 2
e at 10 ÂµM inhibited CYP3A activity by 44%. Kratom extracts at 20 Âµg/mLÂ inhibited CYP3A activity by 82-90%.
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nin-1, 6.0 Â±Â 0.5 ÂµM and 0.074 Â± 0.002 min-1, and 7.3 Â±Â 2.5 ÂµM and 0.17 Â± 0.02 min-1, respectively, for th
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s shown. Note that other reactions besides 7-OH-MTG were also included in the total contribution of metabolism c

igure 2)

not be estimated from the provided figure. 0.01 Âµg/mL: 18 Â± Unknown%0.1 Âµg/mL: 11 Â± 4%1 Âµg/mL: 9Â± 0%

not be estimated from the provided figure. 0.01 Âµg/mL: 25 Â± Unknown%0.1 Âµg/mL: 21 Â± Unknown%1 Âµg/mL

values estimated from Figure 1d. In some cases, SEM could not be estimated from the provided figure. 0.01 Âµg/mL
itragynine levels ranged from 0.01 to 0.04% (0.1 to 0.4 mg/g). Thus, the reported values we have provided a
ated from Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: 43 Â± Unknown
ated from Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: -5 Â± 2%0.2 Î¼M
om Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: 47 Â± Unknown%0.2 Î¼
om Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: 37 Â± Unknown%0.2 Î¼

om Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: 38 Â± Unknown%0.2 Î¼
ated from Figure 2. In some cases, SEM could not be estimated from the provided figure.0.02 Î¼M: -24 Â± 0%0.2 Î¼

Study title
Rate and extent of mitragynine and 7-hydroxymitragynine blood-brain barrier transport and their intra-brain distri
Evaluation of In Vitro Absorption, Distribution, Metabolism, and Excretion (ADME) Properties of Mitragynine, 7-Hy
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Kratom Metabolomics
Effects of mitragynine and 7-hydroxymitragynine (the alkaloids of Mitragyna speciosa Korth) on 4-methylumbellife
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Inhibition of CYP2C9, CYP2D6, and CYP3A activity by Mitragynine and Kratom extracts
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Metabolite profiling and identification of enzymes responsible for the metabolism of mitragynine, the major alkalo
Exploration of cytochrome P450 inhibition mediated drug-drug interaction potential of kratom alkaloids
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The inhibitory effects of mitragynine on P-glycoprotein in vitro
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Evaluation of selected Malaysian medicinal plants on phase I drug metabolizing enzymes, CYP2C9, CYP2D6 and CYP
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P-glycoprotein interactions of novel psychoactive substances - Stimulation of ATP consumption and transport acro
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Quantified metabolite name	Quantified metabolite InChI	ntified metabolite concept ID (or

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(-)-epigallocatechin gallate

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Object metabolite compound InChI **al: Object metabolite compound con**

ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
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ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N
ARQXEQLMMNGFDU-JHZZJYKESA-N

QHSMEGADRFZVNE-UHFFFAOYSA-N
QHSMEGADRFZVNE-UHFFFAOYSA-N
KGVXVPRLBMWZLG-UHFFFAOYSA-N
QHSMEGADRFZVNE-UHFFFAOYSA-N
QHSMEGADRFZVNE-UHFFFAOYSA-N
KGVXVPRLBMWZLG-UHFFFAOYSA-N
QHSMEGADRFZVNE-UHFFFAOYSA-N
JAQUASYNZVUNQP-PVAVHDDUSA-N
JAQUASYNZVUNQP-PVAVHDDUSA-N
JAQUASYNZVUNQP-PVAVHDDUSA-N
QHSMEGADRFZVNE-UHFFFAOYSA-N
QHSMEGADRFZVNE-UHFFFAOYSA-N
QHSMEGADRFZVNE-UHFFFAOYSA-N
JAQUASYNZVUNQP-PVAVHDDUSA-N
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JAQUASYNZVUNQP-PVAVHDDUSA-N
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KGVXVPRLBMWZLG-UHFFFAOYSA-N
JAQUASYNZVUNQP-PVAVHDDUSA-N
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XSEGWEUVSZRCBC-ZVBLRVHNSA-N
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VRXFDHAGFYWGHT-UHFFFAOYSA-N
QHSMEGADRFZVNE-UHFFFAOYSA-N
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RZVAJINKPMORJF-UHFFFAOYSA-N
KGVXVPRLBMWZLG-UHFFFAOYSA-N
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IJQYTHQDUDCJEQ-UHFFFAOYSA-N

CCKWMCUOHJAVOL-UHFFFAOYSA-N	InChi Key generated by ChemDraw 17
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
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IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
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IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin
IWJYWBVPCGUPLO-KOUNZKNHSA-N	AKA d-luciferin

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Precipitant compound unique ingredient identifier	mpound international chem
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	LELBFTMXCIIKKX-QVRQZEMU
	RYENLSMHLCNXJT-CYXFISRXS
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	RYENLSMHLCNXJT-CYXFISRXS
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	LELBFTMXCIIKKX-QVRQZEMU
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	YQEZLKZALYSWHR-UHFFFAO
	LELBFTMXCIIKKX-QVRQZEMU
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	RMRJXGBAOAMLHD-IHFGGW
	RYENLSMHLCNXJT-CYXFISRXS
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	YQEZLKZALYSWHR-UHFFFAO
	RMRJXGBAOAMLHD-IHFGGW
	IAZDPXIOMUYVGZ-UHFFFAO
	LELBFTMXCIIKKX-QVRQZEMU
	IAZDPXIOMUYVGZ-UHFFFAO
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	LELBFTMXCIIKKX-QVRQZEMU
	LELBFTMXCIIKKX-STILVGNPSA
	IXWWTVSMMIIIFZ-JCIDKMOX
	LELBFTMXCIIKKX-QVRQZEMU

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FZYOVNIOYYPUPY-UXKYPCFP
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RYENLSMHLCNXJT-CYXFISRXS
DAXYUDFNWXHGBE-XYEDMT
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RYENLSMHLCNXJT-KPWJTKAC

RYENLSMHLCNXJT-CYXFISRXS
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LELBFTMXCIIKKX-MYLQJJOTS
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JGZKIGWXPPFMRG-CYSPOEIC
VFMMPHCGEFXGIP-UHFFFAC
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RYENLSMHLCNXJT-CYXFISRXS
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JGZKIGWXPPFMRG-CYSPOEIC
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FZYOVNIOYYPUPY-UXKYPCFP

LOUPRKONTZGTKE-LHHVKLH
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QWCJHSGMANYXCW-UHFFFA

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XMAYWYJOQHXEEK-OZXSUG

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LELBFTMXCIIKKX-QVRQZEMU

Precipitant compound description

SA-N

JSA-N

SA-N
VKQSA-N
AOYSA-N
SA-N
JSA-N
JSA-N
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VKQSA-N
SA-N
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VKQSA-N
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OSA-N

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KSA-N

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TIPSA-N

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iGESA-N

lASA-N

AOYSA-N

JSA-N
JSA-N
lASA-N
iGESA-N

AOYSA-N
JSA-N
JSA-N

Internal: Precipitant compound comment	recipitant compound concept ID (omop
	1124300
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	1124300

Often refers to the leaves of M. speciosa

Often refers to the leaves of M. speciosa
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Often refers to the leaves of M. speciosa

Object compound ID	Object compound unique ingredient identifier
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26 R60L0SM5BC
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26 R60L0SM5BC
26 R60L0SM5BC
14 144O8QL0L1
26 R60L0SM5BC
12 7355X3ROTS
12 7355X3ROTS
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14 144O8QL0L1
26 R60L0SM5BC
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12 7355X3ROTS
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26 R60L0SM5BC
25 D9818430MW
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TRUE	http://purl.obolibrary.org/obo/DIDEO_00000058
FALSE	http://purl.obolibrary.org/obo/DIDEO_00000060
FALSE	http://purl.obolibrary.org/obo/DIDEO_00005003

Overview of Supplemental data for Birer, C *et al*. A New Data Repository for Pharmacokinetic Natural Product-Drug Interactions: from Chemical Characterization to Clinical Studies. Drug Metabolism and Disposition

Table S1. Data elements of natural products chemistry studies and of *in vitro* and clinical pharmacokinetic NPDI studies. Data elements are presented for all experiment types of the NaPDI Center repository, for chemical characterization of the material (Cha), metabolomics (Met), *in vitro* enzyme induction (Ind), inhibition (Inh), kinetics (kin), screen (Scr), *in vitro* transporter induction (Ind), inhibition (Inh), kinetics (kin), clinical interaction and pharmacokinetics. Data elements are proposed to be filled "x", are required to be filled "x" or are not available to be filled "-" depending on experiment type.

Table S2. Data in the NaPDI Center repository on cannabis as of April 2020

Table S3. Data in the NaPDI Center repository on kratom as of April 2020

Supplementary material.

1. An example standard operating procedures for NaPDI Repository Data Entry - In vitro Enzyme Inhibition Studies
2. A screen capture video (now audio) showing various features of the NaPDI Repository user interface.