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	Study source type (published report, manuscript *in prep* or *submit* , unpublished data submitted through a NaPDI form)	x	x	x	x	x	x	x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