Table S1 Clinical PK Studies

Ontology	Pharmacogenetics Trial	Drug Interaction Trail
Drugs = SOPHARM_20000	Tamoxifen (TAM)	Midazolam (MDZ, PO 4mg; IV 0.05mg/kg), Ketoconazole (KTZ, PO, 200, 400 mg)
Experiments		
in-vitro		
in-vivo	*in-vivo*	*in-vivo*
Analysis_Method		
Assay	HPLC/MS	HPLC/MS
Dose	SOLTAMOX™, 20mg/day	MDZ PO, IV; KTZ PO
Measurement	month 1, 4, 8, 12	before and 0.5, 0.75, 1, 2, 4, 6, 9 hrs
PK_Parameters	TAM and its metabolites conc	MDZ and KTZ: AUC, AUCR, $t_{1/2}$, and Cmax
Pre-dosing_Conditions		
Sample		
Sample_Size	298	24
Sample_Types	Blood	blood
Stratification	prior chemo, menopausal	
Study_Design		
Bioequivalence_Study		
Dense_Sampling		
Disease-Physiology_PK_Study		
Drug_Interaction_Study		inhibition
Longitudinal	Longitudinal	three-phase crossover
Pharmacogenetics_Study	prospective, single arm	prospective, single arm
Sparse_Sampling		
Steady_State_Study	steady state	
Type_of_PK_Study		
Metabolism		
CYP1_family		
CYP2_family	CYP2D6, 2C9, 2B6	
CYP3_family	CYP3A4/5	CYP3A4/5
CYP4_family		
CYP_other_families		
Subjects		
Disease = DOID_14974	breast cancer	healthy volunteers
Physiology = MP_0000001		
Population = SOPHARM_52000	Caucasian/African American	
Target	ESR1/ESR2	

Note: The annotations are aligned for each row. The left column is the ontology tree presentation. The central and right columns display their corresponding annotations from the paper.

Table S2 *in vitro* PK Study

Ontology	in-vitro study
Drugs ≡ SOPHARM_20000	MDZ, APZ, TZ, CLAR, TAM, DTZ, NIF, BFC, HFC, TEST, E2
Experiments	Compare metabolic capabilities of CYP3A4, 3A5, 3A7
in-vitro	
Experimental_Conditions	
Buffer	sodium phosphate, NADPH, methanol.
NADPH_Source	
Other_Information	
Data_analysis_method	WinNonlin
Dilution	4 fold, 10% methanol (TZ)
Incubation_time	5 min
Microsomal_binding	insect cell (CYP3A)
Number_of_replicates	N/A
Preincubation_time	3min; 6 min
Quantification_method	HPLC, MS, Fluorimetry
kdeg_or_ksyn_of_the_enzyme	CYP3A4/5/7, P450 reductase, b5
Protein	1mol, 6.6mol, 9mol
Protein_Concentration	BD Gentest, PanVera, PanVera
Source	
Non_Recombinant-Enzymes	CYP3A
Recombinant_Enzymes	
Inhibitor_or_Inducer	
Multi_Drug_Experiments	
PK_Parameters	
Emax	
IC50	
KI	
Ki	
Kinact	
Type_of_Interaction	
Single_Drug_Experiments	
PK_Paramaters	
CLint	CL for individual substrates
Km	Km for individual substrates
Vmax	Vmax for individual substrates
Substrate	MDZ, APZ, TZ, CLAR, TAM, DTZ, NIF, BFC, HFC, TEST, E2
in-vivo	
Metabolism	
CYP1_family	
CYP2_family	
CYP3_family	CYP3A4, 3A5, 3A7
CYP4_family	
CYP_4_families_other	

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