

Example Compound Profile Table

For your BPN application, please fill out a compound profile table that summarizes available data for each of the parameters listed in the following example. If a parameter has not been measured, indicate "not done." Name vendors used for any outsourced activities.

Please note: compounds can enter BPN at the Discovery stage (requiring medicinal chemistry) without having any SAR, DMPK, or toxicology data. However, compounds that enter at Development (ready for IND-enabling studies) should have a completed profile table with no apparent liabilities.

Compound identifier/name:

Category	Parameter	Activity	Comments
Chemistry	Molecular weight		
	Aqueous solubility		Indicate method of measurement
	LogP		Note if calculated or determined
	SAR		Indicate # analogs tested, source of analogs, range of activity
Pharmacology	Activity in primary assay		Provide assay name and describe in Research Strategy
	Activity in secondary assay		Provide assay name and describe in Research Strategy
	Selectivity (related family)		Note assays used
	Activity in broad screening panel		Note hits and assoc. activity
	in vivo pharmacology		Note dose, route of admin, animal model; describe study design in Research Strategy
DMPK <i>in vitro</i>	in vitro permeability		Note the assay
	P-glycoprotein transport		Indicate if pgp substrate
	Plasma protein binding		Indicate %
	Microsomal stability		Note species, % remaining, time point
	P450 inhibition		Note CYPs of concern
	CYP induction		Note CYPs of concern
	Metabolite ID		Note unique human metabolites
DMPK <i>in vivo</i>	Brain to plasma		Note species, route of admin
	Bioavailability		Note species, route of admin, dose
	AUC		Note species, route of admin, dose
	MRT		Note species, route of admin, dose
	CL		Note species, route of admin, dose
Toxicology	Cytotoxicity (cells)		Indicate Y/N
	Ames activity		Indicate Y/N
	hERG activity		Indicate potency
	Additional tox activities		Note assays and results