

Table 1. Validated drug-target interactions for Enzyme data.

	Target Annotation	Drugs	Drug Annotation	Database Annotation
hsa1543	cytochrome P450, family 1, subfamily A, polypeptide 1 (EC:1.14.14.1)	D00139'	Methoxsalen (JP16/USP); Oxsooralen (TN)	DrugBank
hsa1571	cytochrome P450, family 2, subfamily E, polypeptide 1 (EC:1.14.13.n7)	D00542	Halothane (JP16/USP/INN);Fluothane (TN)	DrugBank
hsa1200	tripeptidyl peptidase I (EC:3.4.14.9)	D00160	Epsilon-Aminocaproic acid (JAN);Aminocaproic acid (USP/INN);Amicar (TN)	DrugBank
hsa1559	cytochrome P450, family 2, subfamily C, polypeptide 9 (EC:1.14.13.48 1.14.13.49 1.14.13.80)	D00437	Nifedipine (JP16/USP/INN); Adalat (TN); Afeditab CR (TN); Procardia (TN)	DrugBank
hsa5478	peptidylprolyl isomerase A (cyclophilin A) (EC:5.2.1.8)	D00184	Ciclosporin (JP16); Cyclosporine (USP); Gengraf (TN); Neoral (TN);Restasis (TN); Sandimmune (TN)	DrugBank
hsa5150	phosphodiesterase 7A (EC:3.1.4.53)	D00528	Anhydrous caffeine (JP16); Caffeine (USP); Anhydrous caffeine (TN); Respia (TN)	KEGG
hsa5150	phosphodiesterase 7A (EC:3.1.4.53)	D00691	Diprophylline (JAN/INN); Dyphylline (USP); Lufyllin (TN)	DrugBank
hsa4128	monoamine oxidase A (EC:1.4.3.4)	D05458	Phentermine (USAN/INN)	DrugBank
hsa57016	aldo-keto reductase family 1, member B10 (aldose reductase) (EC:1.1.1.2)	D02323	Tolrestat (USAN/INN); Alredase (TN)	DrugBank
hsa1585	CYP11B2, ALDOS, CPN2, CYP11B, CYP11BL, CYPXIB2, P-450C18, P450C18, P450aldo	D00410	Metyrapone (JP16/USP/INN); Metopirone (TN)	DrugBank
hsa50940	phosphodiesterase 11A (EC:3.1.4.35 3.1.4.17)	D00528	Anhydrous caffeine (JP16); Caffeine (USP); Anhydrous caffeine (TN);Respia (TN)	KEGG
hsa4129	monoamine oxidase B (EC:1.4.3.4)	D00947	Linezolid (JAN/USAN/INN); Zyvox (TN)	DrugBank

Table 2. Validated drug-target interactions for Ion channel data.

Targets	Target Annotation	Drugs	Drug Annotation	Database Annotation
hsa1139	cholinergic receptor, nicotinic, alpha 7 (neuronal)	D00499	Pentobarbital (USP/INN); Nembutal (TN)	DrugBank
hsa3767	potassium inwardly-rectifying channel, subfamily J, member 11	D02356	Verapamil (USAN/INN)	DrugBank
hsa778	calcium channel, voltage-dependent, L type, alpha 1F subunit	D01969	Gallopamil hydrochloride (JAN)	KEGG
hsa6331	sodium channel, voltage-gated, type V, alpha subunit	D00538	Zonisamide (JAN/USAN/INN);Excegran (TN)	KEGG
hsa6331	sodium channel, voltage-gated, type V, alpha subunit	D00552	Ethyl aminobenzoate (JP16);Benzocaine (USP/INN);Parathesin (TN)	KEGG
hsa779	calcium channel, voltage-dependent, L type, alpha 1S subunit	D01108	Magnesium sulfate hydrate (JP16);Magnesium sulfate (USP); Magnesium sulfate heptahydrate;Conclyte-Mg (TN)	DrugBank
hsa779	calcium channel, voltage-dependent, L type, alpha 1S subunit	D00438	Nimodipine (USAN/INN); Nimotop (TN); Nymalize (TN)	KEGG
hsa6530	solute carrier family 6 (neurotransmitter transporter), member 2	D02362	Paroxetine (USP/INN); Paroxetine (TN)	DrugBank
hsa1137	cholinergic receptor, nicotinic, alpha 4 (neuronal)	D03365	Nicotine (USP); Habitrol (TN)	DrugBank
hsa6531	solute carrier family 6 (neurotransmitter transporter), member 3	D00394	Trimipramine (USAN/INN)	DrugBank

Table 3. Validated drug-target interactions for Nuclear receptor data.

Targets	Target Annotation	Drugs	Drug Annotation	Database Annotation
hsa2100	estrogen receptor 2 (ER beta)	D00554	Ethinylestradiol (JP16/INN); Ethinyl estradiol (USP); Estinyl (TN)	KEGG
hsa5915	retinoic acid receptor, beta	D00348	Isotretinoin (USP); Absorica (TN);Accutane (TN); Sotret (TN)	KEGG
hsa2100	estrogen receptor 2 (ER beta)	D00898	Dienestrol (USP/INN); DV (TN)	KEGG
hsa5241	progesterone receptor	D00443	Spirolactone (JP16/USP/INN);Aldactone (TN)	DrugBank

Table 4. Validated drug-target interactions for GPCR data.

Targets	Target Annotation	Drugs	Drug Annotation	Database Annotation
hsa1131	cholinergic receptor, muscarinic 3	D00397	Tropicamide (JP16/USP/INN);Mydracyl (TN)	KEGG
hsa1129	cholinergic receptor, muscarinic 2	D00525	Pilocarpine (JAN/USP);Ocuserp pilo-20 (TN)	KEGG
hsa148	adrenoceptor alpha 1A	D00604	Clonidine hydrochloride (JP16/USP); Catapres (TN)	DrugBank
hsa151	adrenoceptor alpha 2B	D02349	Dipivefrin (USAN);Dipivefrine (INN)	KEGG
hsa152	adrenoceptor alpha 2C	D02349	Dipivefrin (USAN);Dipivefrine (INN)	KEGG
hsa152	adrenoceptor alpha 2C	D00563	Mirtazapine (JAN/USAN/INN);Remeron (TN); Reflex (TN)	KEGG
hsa147	adrenoceptor alpha 1B	D00604	Clonidine hydrochloride (JP16/USP); Catapres (TN)	DrugBank
hsa6751	somatostatin receptor 1	D02250	Octreotide acetate (JAN); Octreotide diacetate; Sandostatin (TN)	KEGG
hsa152	adrenoceptor alpha 2C	D00255	Carvedilol (JAN/USAN/INN);Artist (TN); Coreg (TN)	DrugBank
hsa152	adrenoceptor alpha 2C	D00270	Chlorpromazine (USP/INN);Thorazine (TN)	KEGG
hsa1814	dopamine receptor D3	D00283	Clozapine (JAN/USP/INN);Clozaril (TN)	DrugBank
hsa3361	5-hydroxytryptamine (serotonin) receptor 5A, G protein-coupled	D00454	Olanzapine (JAN/USAN/INN);Zyprexa (TN)	DrugBank
hsa1129	cholinergic receptor, muscarinic 2	D00715	Hyoscine methobromide (INN);Methscopolamine bromide;Pamine (TN)	KEGG
hsa1129	cholinergic receptor, muscarinic 2	D01269	Solifenacin succinate (JAN/USAN/INN); Vesicare (TN)	DrugBank
hsa153	adrenoceptor beta 1	D02147	Albuterol (USP); Salbutamol;Proventil (TN)	DrugBank
hsa152	adrenoceptor alpha 2C	D00283	Clozapine (JAN/USP/INN);Clozaril (TN)	DrugBank
hsa1816	dopamine receptor D5	D02340	Loxapine (USAN/INN); Adasuve (TN)	DrugBank
hsa5731	prostaglandin E receptor 1 (subtype EP1), 42kDa	D00079	Dinoprostone (JAN/USP/INN);Cervidil (TN); Prepidil (TN);Prostin E2 (TN)	DrugBank
hsa3356	5-hydroxytryptamine (serotonin) receptor 2A, G protein-coupled	D00136	Haloperidol (JP16/USP/INN);Haldol (TN)	DrugBank
hsa1133	cholinergic receptor, muscarinic 5	D00397	Tropicamide (JP16/USP/INN);Mydracyl (TN)	KEGG
hsa3354	5-hydroxytryptamine (serotonin) receptor 1E, G protein-coupled	D01164	Aripiprazole (JAN/USAN/INN);Abilify (TN)	DrugBank
hsa153	adrenoceptor beta 1	D01386	Ephedrine hydrochloride JP16/USP); Ephedrine hydrochloride (TN)	KEGG
hsa1814	dopamine receptor D3	D00059	Levodopa (JP16/USP/INN);Dopar (TN)	KEGG
hsa1812	dopamine receptor D1	D00136	Haloperidol (JP16/USP/INN);Haldol (TN)	DrugBank
hsa1814	dopamine receptor D3	D00790	Chlorprothixene (JAN/USAN/INN);Taractan (TN)	DrugBank
hsa154	adrenoceptor beta 2, surface	D02358	Metoprolol (USAN/INN)	DrugBank
hsa5732	prostaglandin E receptor 2 (subtype EP2), 53kDa	D02725	Sulprostone (USAN/INN)	KEGG
hsa151	adrenoceptor alpha 2B	D00514	Dexmedetomidine (USAN/INN);Dexdor (TN); Precedex (TN)	KEGG
hsa147	adrenoceptor alpha 1B	D02910	Amiodarone (USAN/INN)	KEGG
hsa151	adrenoceptor alpha 2B	D04375	Guanabenz (USAN/INN)	KEGG