

**S2 Table. Significant DDI-related proteins for cyclosporine, rifampin and theophylline.** DDI-related proteins were manually validated from literatures. “Actual result” indicates whether the identified protein term is true (1) or false (0).

### Cyclosporine

	Protein name	p value	Actual result
	Organic Anion Transporters	0	1
	Cytochrome P-450 CYP3A	0	1
	P-Glycoprotein	0	1
	Cytochrome P-450 Enzyme System	0	1
	Mixed Function Oxygenases	0	0
	Organic Anion Transporters, Sodium-Independent	0	1
	Aryl Hydrocarbon Hydroxylases	0	0
	Oxidoreductases, N-Demethylating	7.18E-14	0
	ATP-Binding Cassette Transporters	1.68E-09	1
	Multidrug Resistance-Associated Proteins	1.88E-08	1
	Membrane Transport Proteins	6.75E-08	1
	Creatine Kinase	3.33E-07	1
	Immunotoxins	8.54E-07	0
	Adenosine Triphosphatases	7.17E-06	0
	Phytohemagglutinins	8.36E-05	1
	Neoplasm Proteins	0.000242148	1
	P-Glycoproteins	0.000268303	1
	Potassium Channels	0.002236825	0
	L-Lactate Dehydrogenase	0.00950413	0
	TOR Serine-Threonine Kinases	0.03366479	0
	Cholesterol, LDL	0.057253658	0
	Receptors, Interleukin-2	0.060776758	0

### Rifampin

	Protein name	p value	Actual result
	Cytochrome P-450 CYP3A	0	1
	Cytochrome P-450 CYP2C8	0	1
	Organic Anion Transporters	0	1
	Cytochrome P-450 Enzyme System	0	1
	P-Glycoprotein	0	1
	Cytochrome P-450 CYP2D6	0	0
	Cytochrome P-450 CYP2C9	2.78E-15	1
	beta-Lactamases	1.99E-14	1
	P-Glycoproteins	4.45E-14	1
	Aryl Hydrocarbon Hydroxylases	5.53E-14	0

Organic Anion Transporters, Sodium-Independent	1.45E-13	1
Cytochrome P-450 CYP2B6	2.77E-11	1
Oxidoreductases, N-Demethylating	2.83E-05	0
Coagulase	0.000269775	0
Mixed Function Oxygenases	0.000325094	0
Glucuronosyltransferase	0.000384339	1
Blood Proteins	0.010634945	0
ATP-Binding Cassette Transporters	0.014110964	1
Alanine Transaminase	0.069149019	0

## Theophylline

	Protein name	p value	Actual result
	Cytochrome P-450 CYP1A2	5.77E-15	1
	Phosphorylases	1.40E-12	1
	Glucosyltransferases	2.13E-10	0
	Cytochrome P-450 Enzyme System	1.34E-07	1
	Receptors, Cholinergic	2.61E-07	0
	Cytochrome P-450 CYP3A	1.64E-05	1
	Phosphoric Monoester Hydrolases	0.000260075	0
	Mixed Function Oxygenases	0.000309117	1
	Receptors, Drug	0.000982719	0
	Pyridoxal Phosphate	0.009505123	0
	Nerve Tissue Proteins	0.027571582	0
	Receptors, Adrenergic	0.038638602	1