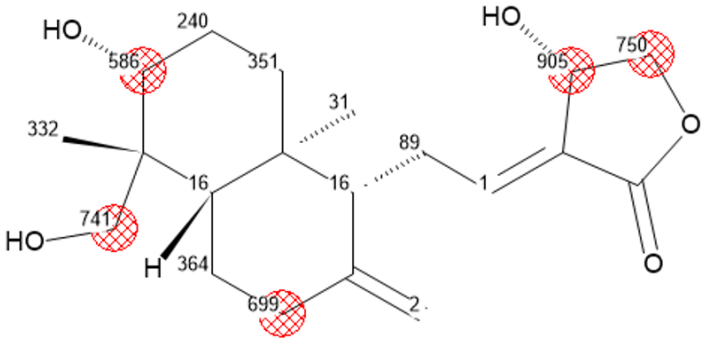
SUPPLEMENTARY DATA

Supplementary 1. Comparison of *in silico* and *in vitro* metabolism analysis of AG

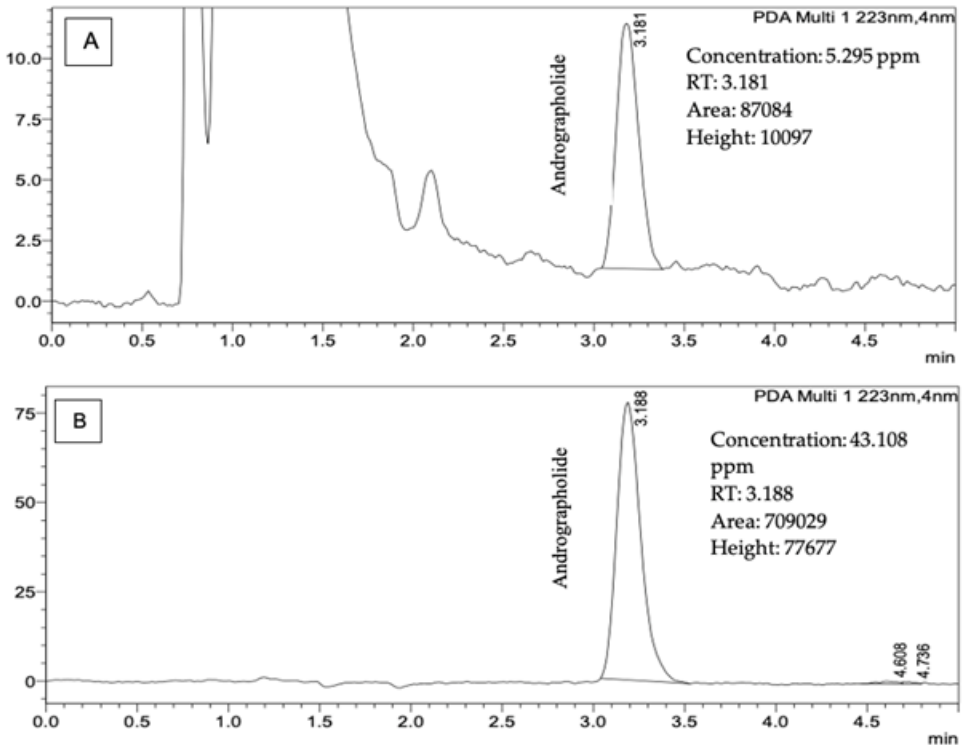
Descriptor	Inhibition		
	In silico	*In vitro*	Positive inhibitor
CYP1A2	No (97%)	Yes: 1 µM (6.7%), 10 µM (10.6%)	Fluvoxamine, 97%
CYP2A6	NA	NA	NA
CYP2B6	No (74%)	Yes: 1 µM (61.7%), 10 µM (64%)	Ticlopidine, 94%
CYP2C8	NA	No: 1 µM (-18.4%), 10 µM (-27.2%)	Quercetin, 79%
CYP2C9	NA	Yes: 1 µM (14.8%), 10 µM (16.8%)	Sulphaphenazol,100%
CYP2C19	No (98%)	No: 1 µM (-13.3%), 10 µM (3.2%)	Fluvoxamine, 96%
CYP2D6	No (59%)	No: 1 µM (-17.2%), 10 µM (-31.5%)	Quinidine, 100%
CYP2E1	NA	NA	NA
CYP3A4	No (76%)	NA	NA
CYP3A4 (Testo)	No (93%)	Yes: 1 µM (33.5%), 10 µM (54.6%)	Ketoconazole, 99%
CYP3A4 (MDZ)	No (62%)	No: 1 µM (-13.3%), 10µM (-23.4%)	Ketoconazole, 98%

NA= Not applicable

Supplementary 2. The red circles show the predicted site of metabolism for CYP3A4



Supplementary 3. HPLC chromatogram of (A) *A. paniculata* aqueous extract; (B) Standard, andrographolide. RT= retention time obtained from HPLC system of Waters 2690 Alliance Separation Module with Zorbax Eclipse XDB-C18 (4.6 mm × 150 mm × 5 µm).



Supplementary 4. Percentage of inhibition (%) by AG against CYP450 isomers based LC-MS/MS analysis. Negative value indicates that no inhibition was observed.