

Supporting Information (SI)

A new calibration curve calculation method for absolute quantification of drug
metabolizing enzymes in human liver microsomes by stable isotope dilution mass
spectrometry

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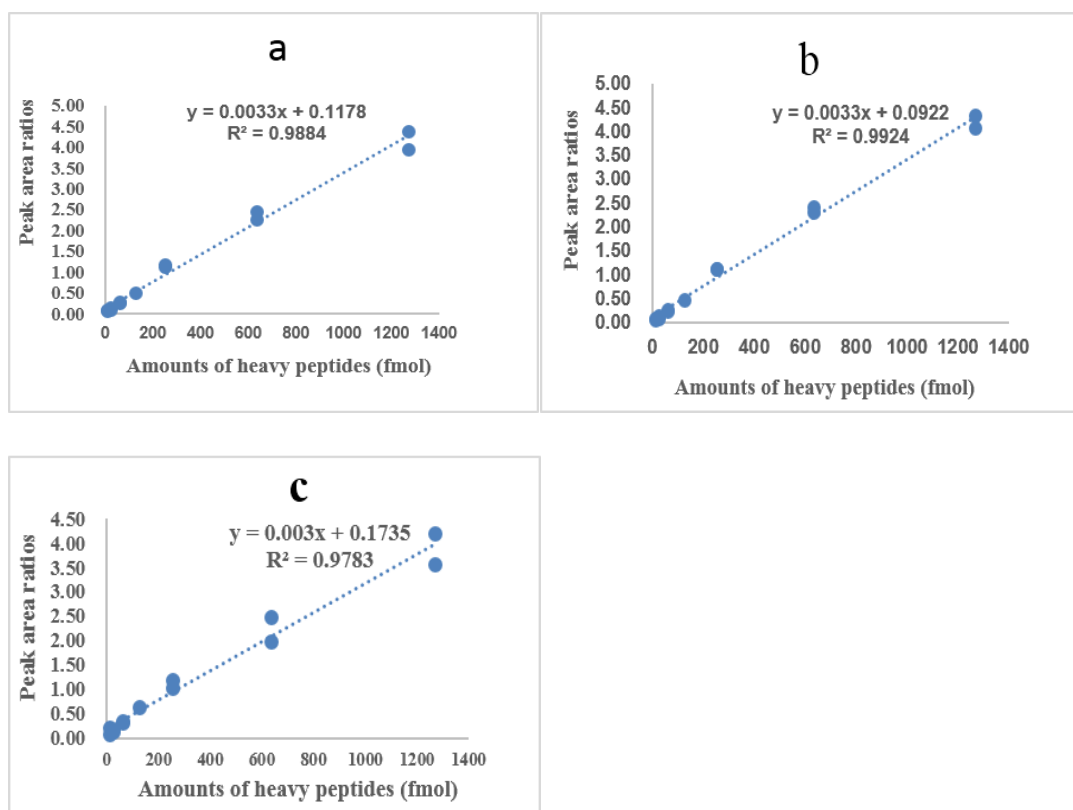


Fig. S1 Linear curves of three transitions from the peptide ASGNLIPQEK of CYP1A2

a, transition 528.8/507.3; b, transition 528.8/620.4; c, transition 528.8/904.5.

Table S1 MS parameter, linearity and sensitivity of 37 tryptic peptides of 21cytochrome P450 Enzymes

protein	peptide sequence	Q1 ^a	Q3 ^b	linear equations	correlation coefficient (R ²)	LOQ (fmol)	dynamic concentration Range (fmol)
CYP 1A2	IGSTPVLVLSR	571.4	783.5	$y = 1.3222x - 0.2393$	0.9774	5	5~1000
			1028.6	$y = 1.3415x - 0.1876$	0.9792	5	5~1000
			587.4	$y = 1.1944x - 0.1947$	0.9874	5	5~1000
	ASGNLIPQEK	528.8	501.3	$y = 0.9542x + 0.1098$	0.9885	5	5~1000
			614.4	$y = 0.9694x + 0.0833$	0.9923	5	5~1000
			898.5	$y = 0.8759x + 0.169$	0.9787	5	5~1000
CYP 2A6	GYGVVFSNGER	592.8	709.3	$y = 1.4391x - 0.2985$	0.9936	5	5~1000
			808.4	$y = 1.598x - 0.4395$	0.9928	5	5~1000
			562.3	$y = 1.4451x - 0.3705$	0.9854	5	5~1000
	GTGGANIDPTFFLSR	776.9	867.5	$y = 0.5117x - 0.1514$	0.997	5	5~1000
			982.5	$y = 0.4755x - 0.3245$	0.9774	5	5~1000
			1209.6	$y = 0.5809x - 0.3949$	0.9755	5	5~1000
	GTEVYPMLGSLVR	711.4	872.5	$y = 1.0378x - 0.7843$	0.9526	5	5~1000
			1035.6	$y = 0.9858x - 0.6752$	0.9638	5	5~1000
			531.3	$y = 0.9339x - 0.7112$	0.9539	5	5~1000
CYP 2B6	IAMVDPFFR	548.3	780.4	$y = 1.2089x + 1.2349$	0.97	5	5~1000
			681.3	$y = 1.4772x - 0.8972$	0.98	5	5~1000
	DLIDTYLLHMEK	745.9	657.3	$y = 1.004x - 1.5898$	0.9525	5	5~1000
			770.4	$y = 1.4785x - 1.2692$	0.9525	5	5~1000
			781.4	$y = 0.677x - 0.5343$	0.9515	5	5~1000
CYP 2C8	EALIDNGEEFSGR	718.8	1010.4	$y = 0.9959x - 0.0843$	0.9731	5	5~1000
			895.4	$y = 1.0669x - 0.0074$	0.9624	5	5~1000
			866.5	$y = 1.0197x - 0.1496$	0.9829	5	5~1000
	DQNFLTLMK	555.2	492.3	$y = 1.3279x - 0.3488$	0.963	5	5~1000
			605.4	$y = 1.1096x - 0.3241$	0.9893	5	5~1000
			444.3	$y = 1.9783x - 0.8042$	0.9832	5	5~1000
	VQEEIDHVIGR	432.3	345.2	$y = 0.8736x - 0.1752$	0.9633	5	5~1000
			581.4	$y = 0.9853x - 0.3389$	0.9846	5	5~1000
			585.3	$y = 1.2205x - 0.4345$	0.9652	5	5~1000
CYP 2C9	GIFPLAER	451.8	732.4	$y = 1.1742x - 0.1122$	0.9961	5	5~1000
			488.3	$y = 1.1436x - 0.0878$	0.9918	5	5~1000
			668.4	$y = 1.2403x - 0.1458$	0.9974	5	5~1000
	SHMPYTDAAVVEVQR	590.3	767.4	$y = 0.6932x - 0.1204$	0.9921	20	20~1000
			937.5	$y = 0.6363x - 0.0951$	0.9561	20	20~1000
			1111.5	$y = 0.611x - 0.0706$	0.9719	20	20~1000

CYP2C19	NLAFMESDILEK	705.4	964.5	$y = 1.0988x + 1.8411$	0.9869	5	5~1000
			1182.6	$y = 1.0205x + 1.1528$	0.9515	5	5~1000
			861.5	$y = 1.4187x + 0.4451$	0.9943	5	5~1000
CYP 2E1	EAHFLLEALR	599.9	714.5	$y = 1.700x - 0.677$	0.9903	5	5~1000
			601.4	$y = 1.726x - 0.679$	0.9912	5	5~1000
			1121.6	$y = 1.889x - 0.869$	0.9903	5	5~1000
	FITLVPSNLPHEATR	848	1220.6	$y = 1.402x - 0.348$	0.9943	5	5~1000
			476.3	$y = 1.230x - 0.225$	0.9942	5	5~1000
			542.3	$y = 1.412x - 0.361$	0.9869	5	5~1000
CYP 2D6	DLTEAFLAEMEK	698.9	607.3	$y = 1.534x - 0.564$	0.9886	20	20~1000
			720.4	$y = 1.415x - 0.337$	0.9932	10	10~1000
			735.4	$y = 1.369x - 0.365$	0.999	10	10~1000
	DIEVQGFR	482.2	606.3	$y = 1.045x - 0.034$	0.9971	5	5~1000
			507.3	$y = 1.051x - 0.001$	0.9991	5	5~1000
			843.5	$y = 1.106x - 0.202$	0.9969	5	5~1000
CYP 3A4	GVVVMIPSYALHR	721.4	1087.6	$y = 0.807x + 0.338$	0.9968	5	5~1000
			956.5	$y = 0.708x + 0.845$	0.9846	5	5~1000
			721.4	$y = 0.854x + 0.030$	0.9947	5	5~1000
CYP 3A5	DTINFLSK	469.3	608.3	$y = 0.7761x + 0.279$	0.9778	5	5~1000
			783.5	$y = 0.9447x + 0.054$	0.9787	5	5~1000
UGT 1A1	DGAFYTLK	457.7	671.4	$y = 1.0134x + 0.0377$	0.9971	5	5~1000
			524.3	$y = 0.9989x + 0.0033$	0.9961	5	5~1000
			361.2	$y = 0.9818x - 0.0314$	0.9901	5	5~1000
UGT 1A3	YLSIPTVFFLR	678.4	879.5	$y = 2.672x - 1.670$	0.999	5	5~1000
UGT 1A4	YIPCDLDFK	585.8	894.4	$y = 1.3271x - 0.2377$	0.9706	5	5~1000
			637.3	$y = 1.1464x - 0.0774$	0.9903	5	5~1000
			797.3	$y = 0.8891x + 0.0416$	0.9679	5	5~1000
	GTQCPNPSSYIPK	724.8	1002.5	$y = 1.3837x - 0.1521$	0.989	5	5~1000
			791.4	$y = 0.989x + 0.0365$	0.9657	5	5~1000
			905.5	$y = 0.8537x + 0.1432$	0.9621	5	5~1000
UGT 1A6	DIVEVLSDR	523.3	817.4	$y = 1.6296x - 0.3944$	0.991	5	5~1000
			718.4	$y = 1.9613x - 0.8129$	0.9941	5	5~1000
			589.3	$y = 1.9597x - 0.8321$	0.9847	5	5~1000
	SFLTAPQTEYR	656.8	793.4	$y = 1.6564x - 0.6652$	0.9476	5	5~1000
			965.5	$y = 1.4314x - 0.0492$	0.9554	5	5~1000
			864.4	$y = 1.6163x - 0.585$	0.9437	5	5~1000
UGT 1A9	AFAHAQWK	479.7	532.3	$y = 1.363x - 0.220$	0.9969	5	10~1000
			740.4	$y = 1.234x - 0.270$	0.9855	5	10~1000
			669.3	$y = 1.307x - 0.229$	0.9991	5	10~1000
UGT 2B4	TILDELVQR	543.8	872.5	$y = 0.9932x - 0.0095$	0.9988	5	5~1000
			644.4	$y = 1.0266x - 0.0235$	0.9985	5	5~1000
			759.4	$y = 1.065x - 0.0565$	0.9986	5	5~1000
	FSPGYAIEK	506.3	777.4	$y = 1.0321x - 0.0036$	0.9955	5	5~1000
			680.4	$y = 0.9443x + 0.0354$	0.9969	5	5~1000

UGT 2B7	TILDELIQR	550.8	773.4	y=0.9867x-0.0009	0.9443	5	5~1000
			886.5	y=1.0485x-0.0177	0.9995	5	5~1000
			773.4	y=0.9867x-0.0009	0.9991	5	5~1000
			658.4	y=1.0397x-0.0134	0.9993	5	5~1000
	IEIYPTSLTK	582.8	646.4	y=0.9522x+0.0199	0.9975	5	5~1000
			922.5	y=1.0412x-0.0082	0.9976	5	10~1000
			809.4	y=1.0329x-0.0059	0.9987	5	10~1000
			372.2	y=0.9527x-0.0011	0.9991	5	10~1000
UGT2B10	HSGGFIFPPSYVPVMSK	975.0	1026.6	y=1.0169x-0.0076	0.9975	5	5~1000
			660.4	y=1.0702x-0.1344	0.9983	5	20~1000
			1106.6	y=0.7467x+0.2856	0.9932	5	20~1000
UGT2B11	FEVYPTSLTK	592.8	1203.6	y=1.1086x-0.0877	0.9992	5	20~1000
			809.4	y=0.8885x+1.7022	0.9932	5	5~1000
			549.3	y=1.3402x-0.3402	0.9878	5	5~1000
UGT2B15	SVINDPVYK	517.8	848.5	y=0.926X-0.0278	0.9955	5	5~1000
			506.3	y=1.2216x-0.0217	0.9931	5	5~1000
			735.4	y=0.9725x-0.0175	0.9921	5	5~1000
	FSVGYTFEK	539.3	744.4	y=0.9373x+0.0231	0.9889	5	5~1000
			843.4	y=0.9569x+0.0094	0.9953	5	5~1000
			930.5	y=1.1669x-0.0137	0.9972	5	5~1000
			760.4	y=1.189x-0.037	0.994	5	5~1000
POR ^a	GVATNWLR	458.8	689.4	y=1.176x-0.052	0.9988	5	5~1000
			588.3	y=1.322x-0.09	0.9876	5	5~1000
	FAVFGLGNK	476.8	488.3	y=0.9853x+0.0099	0.999	5	5~1000
			635.4	y=1.0393x-0.0024	0.999	5	5~1000
			734.4	y=0.9519x+0.0227	0.999	5	5~1000

^a cytochrome P450 oxidoreductase