

Identification of the cytochrome P450 enzymes involved in the oxidative metabolism of trantinterol
using ultra high-performance liquid chromatography coupled with tandem mass spectrometry

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Table S1 Summary of accuracy, intra- and inter-assay precision from QCs in human liver microsomes and cDNA-expressed P450 enzymes.

Analytes	Added <i>C</i> (ng/mL)	Found <i>C</i> (ng/mL)	Relative error (%)	Intra-run <i>RSD</i> (%)	Inter-run <i>RSD</i> (%)
In HLMs					
M1	9.640	9.642	0.0	5.8	9.6
	23.13	25.32	9.5	3.9	3.6
	241.0	243.2	0.9	6.0	4.9
	2410	2090	-13	2.7	7.1
M2	1.843	1.830	-0.7	5.1	12
	3.072	3.262	6.2	6.7	11
	32.77	34.13	4.2	2.9	5.7
	384.0	365.6	-4.8	2.9	8.2
In CYPs					
M1	9.640	9.824	1.9	5.1	8.5
	23.13	25.89	12	2.5	10
	241.0	255.4	6.0	3.3	3.4
	2410	2115	-12	2.9	1.2
M2	1.843	1.848	0.3	8.7	11
	3.072	3.084	0.4	5.9	3.4
	32.77	34.44	5.1	3.1	5.2
	384.0	361.4	-5.9	5.1	8.3

Table S2 Stabilities of M1 and M2 in human liver microsomes and cDNA-expressed P450 enzymes.

Storage conditions	Analytes	Added <i>C</i> (ng/mL)	Found <i>C</i> (ng/mL)	<i>RE</i> (%)	<i>RSD</i> (%)
In HLMs					
Post-preparative (4°C for 12 h)	M1	23.13	25.36	9.7	7.4
		2410	2105	-13	2.4
	M2	3.072	2.809	-8.6	10
		384.0	373.5	-2.7	6.1
Incubation for 40 min	M1	23.13	25.65	11	3.5
		2410	2057	-15	0.3
	M2	3.072	3.145	2.4	6.0
		384.0	358.9	-6.5	3.0
In CYPs					
Post-preparative (4°C for 12 h)	M1	23.13	26.36	14	1.8
		2410	2117	-12	1.5
	M2	3.072	3.026	-1.5	1.2
		384.0	349.3	-9.0	5.6
Incubation for 40 min	M1	23.13	25.93	12	3.1
		2410	2195	-8.9	1.3
	M2	3.072	3.117	1.5	6.0
		384.0	381.9	-0.5	4.6