Supplementary Table 2A: Optimised mass spectrometric fragmentation parameters for flurbiprofen, hydroxy-flurbiprofen and internal standard probenecid in negative mode $[M - H]^-$

Analyte	CYP probe	Q1 (m/z)	Q3 (m/z)	DP (V)	CE (V)	CXP (V)
Flurbiprofen	**CYP2C9**	243.20	199.30	-12	-14	-12
Hydroxyflurbiprofen		259.20	215.20	-40	-11	-4
Internal Standard						
Probenecid		284.30	240.30	-50	-24	-10

CYP = Cytochrome P450; m/z – mass to charge ratio; DP = declustering potential in volts; CE = collision energy in volts; collision cell exit potential in volts.

Supplementary Table 2B: Optimised mass spectrometric fragmentation parameters for analytes and internal standard imipramine in positive mode $[M+H]^+$

Analyte	Probe	Q1 (m/z)	Q3 (m/z)	DP (V)	CE (V)	CXP (V)
Fexofenadine	**P-gp**	502.7	466.6; 484.7	100	38	12
Caffeine	**CYP1A2**	195.3	138.2	20	25	6
Paraxanthine		181.1	124.2	70	27	5
Bupropion	**CYP2B6**	240.4	131.3	20	50	11
Hydroxybupropion		256.4	103.1	50	52	3
Omeprazole	**CYP2C19**	346.3	198.1	25	30	10
Hydroxyomeprazole		362.1	214.4	50	15	10
Dextromethorphan	**CYP2D6**	272.4	147.4; 171.5	90	50	10
Dextrorphan		258.4	157.2	80	45	4
Midazolam	**CYP3A4**	326.3	291.4	80	35	14
Hydroxymidazolam		342.2	324.1	89	29	18
Internal Standard						
Imipramine		281.5	86.1	50	50	10

P-gp = permeability glycoprotein; CYP = Cytochrome P450; m/z – mass to charge ratio; DP = declustering potential in volts; CE = collision energy in volts; collision cell exit potential in volts.