

Selective inhibition of cytochrome P450 2D6 by sarpogrelate and its active metabolite, M-1, in human liver microsomes. Doo-Yeoun Cho, Soo Hyeon Bae, Joeng Kee Lee, Yang Weon Kim, Bom-Taeck Kim, Soo Kyung Bae. *Drug Metabolism and Disposition*

Supplemental Table 1. Optimized mass parameters for the detection of metabolites of the nine P450-selective substrates and internal standard using cocktail assays on the API5500 Qtrap instruments

P450s	Substrates	Concentration (μM)	Metabolites	Transitions (m/z)	ESI mode	DP (eV)	CE (eV)
1A2	Phenacetin	50	Acetaminophen	152 / 110	+	50	20
2A6	Coumarin	5	7-Hydroxycoumarin	161 / 105	-	-90	-30
2B6	Bupropion	50	6-Hydroxybupropion	256 / 238	+	140	20
2C8	Rosiglitazone	1	p-Hydroxyrosiglitazone	374 / 151	+	60	30
2C9	Tolbutamide	100	4-Hydroxytolbutamide	285 / 104	-	-20	-40
2C19	S-Mephenytoin	100	4'-Hydroxymepheytoin	233 / 190	-	-45	-20
2D6	Dextromethorphan	5	Dextrophan	258 / 157	+	190	50
2E1	Chlorzoxazone	50	6-Hydroxychlorzoxazone	184 / 120	-	-100	-40
3A	Midazolam	5	1'-Hydroxymidazolam	342 / 203	+	20	40
Internal standard	Chlorpropamide			277 / 111	+	120	20
				275 / 190	-	-80	-50

ESI, electrospray ionization; DP, declustering potential; CE, collision energy.

The Optimized ion spray voltage and temperature were set at ±5500 V and 500°C, respectively.