Mechanisms of Herb-Drug Interactions Involving Cinnamon and Cytochrome P450 2A6: Focus on Time-dependent Inhibition by Cinnamaldehyde and 2-Methoxycinnamaldehyde

Michael J. Espiritu, Justin Chen, Jaydeep Yadav, Michael Larkin, Robert D. Pelletier, Jeannine M. Chan, Jeevan B. GC, Senthil Natesan, and John P. Harrelson

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Supplemental Material 4 LCMS MetID Conditions

LC/MS Conditions for Metabolite Identification

The LC/MS system was composed of an UHPLC (Waters I Class, Milford, MA) and a hybrid quadrupole/time of flight mass spectrometer (AB SCIEX 5600 TripleTOF, Applied Biosystems, Framingham, MA). Data were collected by Analyst TF (version 1.7.1, Applied Biosystems, Framingham, MA), analyzed with PeakView (version 2.2, Applied Biosystems) and Metabolite Pilot (version 2.0.2, Applied Biosystems) and integrated with MultiQuant (version 3.0.2, Applied Biosystems). The details were as follows:

LC Conditions	
Column:	Waters Sunfire C_{18} 2.1 × 150 mm, 5 µ (Milford, MA)
Column Temperature:	Ambient
Needle Wash:	Acetonitrile/methanol
Mobile Phases:	(A) 0.1% formic acid in water
	(B) 0.1% formic acid in acetonitrile
Gradient:	(B) 0% (0 - 1 min), 100% (14-15 min), 0% (15.1-20 min)
Flow Rate:	500 µL/min
Sample Tray Temperature:	4°C
Sample Injection Volume:	10 µL
MS Conditions	
Ionization Mode	Positive
Curtain Gas:	35
Temperature:	600°C
GAS1:	60
GAS2:	60
ISVF:	4500 V
Survey Scan Settings:	
Scan Range:	50-2000 m/z
Accumulation Time:	0.1 sec
DP:	100
CE:	5
CES:	0
IDA Settings:	
Maximum Scans per cycle:	4 (Product Ion)
Scan Range:	50-2000 m/z
Accumulation Time:	0.1 sec

DP:	100
CE:	40
CES:	15
IDA Trigger Type:	Mass Defect Filter and Largest Peak
Mass Defect Filters:	
	80 mDa error/500 Da window with $C_{10}H_{10}O_2$
Exclude previous ions:	1 sec
Minimum CPS for trigger:	300