

Table S1. Inclusion lists for liquid chromatography-high-resolution tandem mass spectrometry analysis of human hepatocyte incubates

Composition change	Elemental composition	[M+H] ⁺ , <i>m/z</i>	[M-H] ⁻ , <i>m/z</i>	Reference transformation
-	C ₁₄ H ₂₀ N ₂ O	233.1648	231.1503	None (parent)
+3O +S	C ₁₄ H ₂₀ N ₂ O ₄ S	313.1216	311.1071	Sulfation
+6C +8H +6O	C ₂₀ H ₂₈ N ₂ O ₇	409.1969	407.1824	Glucuronidation
+C +2H	C ₁₅ H ₂₂ N ₂ O	247.1805	245.1659	Methylation
+O	C ₁₄ H ₂₀ N ₂ O ₂	249.1598	247.1452	Hydroxylation
-3C -6H	C ₁₁ H ₁₄ N ₂ O	191.1179	189.1033	<i>N</i> -Depropylation
-C -2H	C ₁₃ H ₁₈ N ₂ O	219.1492	217.1346	<i>N</i> -Demethylation
-2H +2O	C ₁₄ H ₁₈ N ₂ O ₃	263.1390	261.1245	Carboxylic acid formation (ω -alkyl)
-4C -9H -N +O	C ₁₀ H ₁₁ NO ₂	178.0863	176.0717	<i>N</i> -Dealkylation to alcohol
-4C -11H -N +O	C ₁₀ H ₉ NO ₂	176.0706	174.0561	<i>N</i> -Dealkylation to aldehyde
-2H	C ₁₄ H ₁₈ N ₂ O	231.1492	229.1346	Dehydrogenation
-2H +O	C ₁₄ H ₁₈ N ₂ O ₂	247.1441	245.1296	Oxidation
+4O +S	C ₁₄ H ₂₀ N ₂ O ₅ S	329.1166	327.1021	Sulfation + Hydroxylation
-3C -6H +3O +S	C ₁₁ H ₁₄ N ₂ O ₄ S	271.0747	269.0602	Sulfation + <i>N</i> -Depropylation
-C -2H +3O +S	C ₁₃ H ₁₈ N ₂ O ₄ S	299.1060	297.0914	Sulfation + <i>N</i> -Demethylation
-2H +5O +S	C ₁₄ H ₁₈ N ₂ O ₆ S	343.0958	341.0813	Sulfation + Carboxylic acid formation (ω -alkyl)
+6C +8H +7O	C ₂₀ H ₂₈ N ₂ O ₈	425.1918	423.1773	Glucuronidation + Hydroxylation
+3C +2H +6O	C ₁₇ H ₂₂ N ₂ O ₇	367.1500	365.1354	Glucuronidation + <i>N</i> -Depropylation
+5C +6H +6O	C ₁₉ H ₂₆ N ₂ O ₇	395.1813	393.1667	Glucuronidation + <i>N</i> -Demethylation
+6C +6H +8O	C ₂₀ H ₂₆ N ₂ O ₉	439.1711	437.1566	Glucuronidation + Carboxylic acid formation (ω -alkyl)
+C +2H +O	C ₁₅ H ₂₂ N ₂ O ₂	263.1754	261.1609	Methylation + Hydroxylation
-2C +4H	C ₁₂ H ₁₆ N ₂ O	205.1336	203.1190	Methylation + <i>N</i> -Depropylation
+C +2O	C ₁₅ H ₂₀ N ₂ O ₃	277.1547	275.1401	Methylation + Carboxylic acid formation (ω -alkyl)
+2O	C ₁₄ H ₂₀ N ₂ O ₃	265.1547	263.1401	Dihydroxylation
-2C -6H +2O	C ₁₂ H ₁₄ N ₂ O ₃	235.1077	233.0932	<i>N</i> -Depropylation + <i>N</i> -Carboxylation
-C -2H +O	C ₁₃ H ₁₈ N ₂ O ₂	235.1441	233.1296	<i>N</i> -Demethylation+ Hydroxylation
+C +2H +4O +S	C ₁₅ H ₂₂ N ₂ O ₅ S	343.1322	341.1177	Sulfation + Methylation + Hydroxylation
+7C +10H +7O	C ₂₁ H ₃₀ N ₂ O ₈	439.2075	437.1929	Glucuronidation + Methylation + Hydroxylation