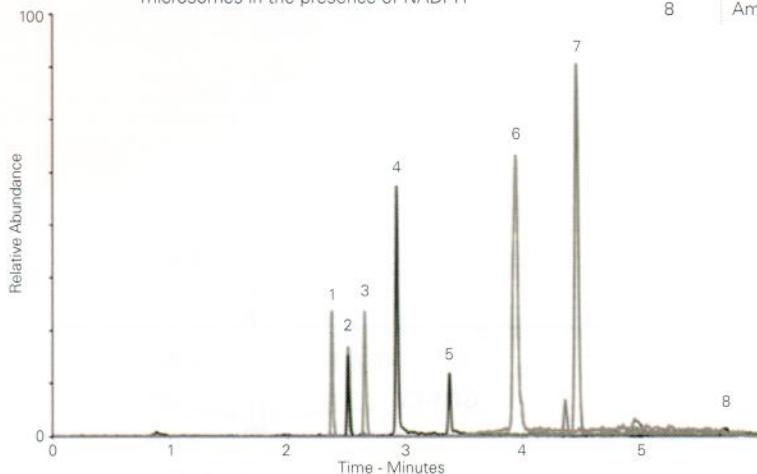


Conditions

Column: ACE 5 C18-300
Dimensions: 150 x 4.6 mm
Part Number: ACE-221-1546
Mobile Phase: 0.1% (v/v) formic acid in H₂O/MeCN (35:65 v/v)
Flow Rate: 0.4 mL/min
Injection: 15 µL
Temperature: 21 °C
Detection: Agilent 6410 triple quad MS
 ESI in positive ion mode
 Full scan MS and MS/MS data obtained
Sample: *In vitro* incubation of amoxicillin with human liver microsomes in the presence of NADPH

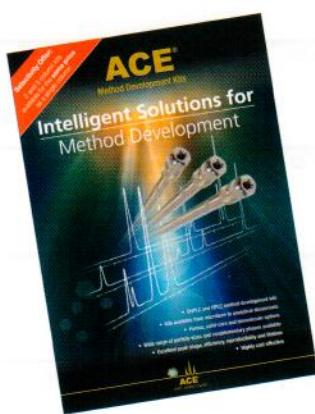
Peak	Analyte	[M+H] ⁺	Elemental Composition	Metabolic Reaction
1	M1	382	C ₁₆ H ₂₀ N ₃ O ₆ S	Hydroxylation
2	M2	379	C ₁₇ H ₁₉ N ₂ O ₆ S	Oxidative deamination
3	M3	382	C ₁₆ H ₂₀ N ₃ O ₆ S	Oxidation of aliphatic chain
4	M4	380	C ₁₆ H ₁₈ N ₃ O ₆ S	Oxidation of aliphatic chain
5	M5	396	C ₁₆ H ₂₀ N ₃ O ₇ S	Oxidation of aliphatic chain
6	M6	322	C ₁₅ H ₁₉ N ₃ O ₃ S	Decarboxylation
7	M7	542	C ₂₅ H ₂₈ N ₃ O ₁₁ S	Glucuronidation
8	Amoxicillin	366	C ₁₆ H ₂₀ N ₃ O ₅ S	



Szultka M, Krzeminski R, Jackowski M, Buszewski B. (2014) Identification of *in vitro* Metabolites of Amoxicillin in Human Liver Microsomes by LC-ESI/MS, Chromatographia, 77 , 1027-1035. doi 10.1007/s10337-014-2648-2

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