

Supplementary Materials

Identification of the impurities in chloroephedrine samples by HPLC-IT/TOF-MS and preparation of chloroephedrine standard

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Table S1. Characterization summary of the impurities identified in chloroephedrine samples

Identity	R _t /min	Intensity/10 ⁶ cps	Molecular formula	Experimental mass (m/z)	Theoretical mass (m/z)	Error/mDa	Degree of unsaturation	Fragment ion
Chloroephedrine	6.869	7.203	C ₁₀ H ₁₄ ClN	183.0885	183.0821	-6.43	4	184.1046 (C ₁₀ H ₁₅ ClN ⁺) 148.0938 (C ₁₀ H ₁₄ N ⁺) 133.0389 (C ₉ H ₁₁ N ⁺) 117.0526 (C ₉ H ₉ ⁺)
Impurity 1	7.692	2.758	C ₁₀ H ₁₄ ClN	183.0860	183.0821	-3.99	4	184.1021 (C ₁₀ H ₁₅ ClN ⁺) 148.1028 (C ₁₀ H ₁₄ N ⁺) 133.0650 (C ₉ H ₁₁ N ⁺) 117.0712 (C ₉ H ₉ ⁺)
Impurity 2	19.420	3.706	C ₁₉ H ₂₂ ClN	299.1512	299.1568	5.61	9	300.1043 (C ₁₉ H ₂₃ ClN ⁺) 264.2059 (C ₁₉ H ₂₂ N ⁺)

R_t: retention time

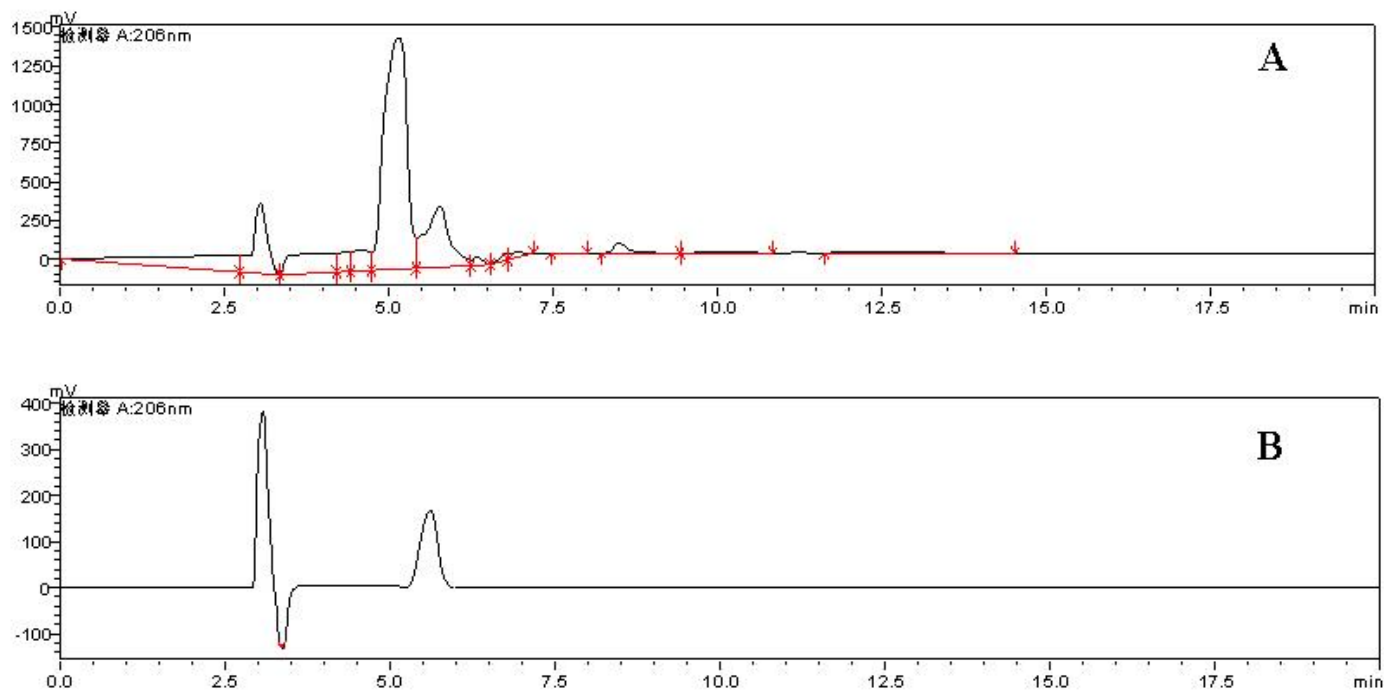


Figure S1. Analytical HPLC chromatogram of chlorephedrine sample (A) and (1R, 2S)-β-chloro-methamphetamine (B)
 Chiral separation conditions: a chiralpak AD-H column (250 mm×4.6 mm, 5 μm, DAICEL, Osaka, Japan);
 Column temperature was 25℃; Mobile phase was *n*-hexane:2-propanol:trifluoroacetic acid:triethylamine=92:8:0.1:0.05;
 Flow rate was 1.0 mL/min.