

液相色谱: Agilent 1260 或者 1290 Infinite II

色谱柱: 方法一: C<sub>18</sub>, 4.6 mm × 250 mm, 5 μm, Luna, Phenomenex

方法二: C<sub>18</sub>, 3.0 mm × 150 mm, 3 μm, packed by ourselves, materials from GALAK

进样量: 200 μL (方法一), 100 μL (方法二)

紫外检测器: DAD, 60 mm Max-Light Cartridge Cell (G4212-60007)

**Table S1.** Gradient elution parameters for UHPLC (Method 1: using a 4.6 mm ID column with a flow rate of 1.0 mL min<sup>-1</sup>)

Time (min)	Acetonitrile + 0.05% trifluoroacetic acid (%)	H <sub>2</sub> O + 0.05% trifluoroacetic acid (%)
0	30	70
3	30	70
25	80	20
26	30	70
30	30	70

**Table S2.** Gradient elution parameters for UHPLC (Method 2: using a 3.0 mm ID column (C<sub>18</sub>) with a flow rate of 0.5 mL min<sup>-1</sup>)

Time (min)	Acetonitrile + 0.05% trifluoroacetic acid (%)	H <sub>2</sub> O + 0.05% trifluoroacetic acid (%)
0	20	80
2	20	80
17	75	25
18	20	80
23	20	80

**Table S3.** The detector parameters and the retention times for probe analysis with UHPLC.

Compound	Detection wavelength	Retention Time (Method 1)	Retention Time (Method 2)
BA	230 nm	11.2 min	9.2 min
<i>p</i> CBA	240 nm	15.5 min	11.9 min
TMBA	225 nm	16.5 min	12.6 min
NB	266 nm	17.3 min	13.1 min
TMP	220 nm $E_x = 230 \text{ nm}, E_m = 325 \text{ nm}^*$	19.8 min	14.9 min

\* A fluorescence detector (FLD) was employed when the [TMP] is lower than 0.2  $\mu\text{M}$ .