Table 1. Multiple reaction monitoring (MRM) condition of HBCDs using UPLC/MS/MS

Parameter	Native HBCDs	$^{13}C_{12}$-HBCDs	d18-HBCDs
Parent ion (m/z)	640.7	652.8	657.8
Daughter ion (m/z)	79 and 81		
Cone voltage (V)	25		
Collision energy (eV)	15		

Table 2. Mobile phase gradient conditions for UPLC/MS/MS analysis of HBCDs

Time (min)	#1		#2		#3	
	A (%)	B (%)	A (%)	B (%)	A (%)	B (%)
Initial	10	90	50	50	80	20
5	10	90	50	50	80	20
14	95	5	95	5	95	5
20	10	90	50	50	80	20

Table 3. Optimized UPLC/MS/MS for analyzing HBCDs isomers

Analyzer	UPLC (Ultra performance liquid chromatography, Waters		
Column	Waters Acquity BEH C18 column (2.1 × 100 mm, 1.7 μm)		
Injection	5 μL		
Column temperature	40℃		
Mobile phase	(A) Methanol/ACN (7:3, v/v), (B) 10 mM AA (in DIW)		
Concentration gradient	Time (min)	Methanol (%)	10 mM of Ammonium acetate
	Initial	5	95
	6	20	80
	13	100	0
	15	100	0
	17	5	95
	20	5	95
Total running time	20 min		
Mass analyzer	Waters Xevo TQ-S		
Ion source	Electrospray negative: ESI (-)		
Gas and flow rate	Nitrogen (7 bar), 800 L/h		
Vaporizer temp.	350℃		
Detection method	Multiple Reaction Monitoring (MRM)		