

Supplementary Material

Table S1. Detailed information of ZEN-14G and major metabolites including precursor ions and corresponding product ions, collision energy, linear equation, and sensitivity.

Compound	Precursor Ion (<i>m/z</i>)	Product Ion (<i>m/z</i>)	CE (eV)	Elemental Composition	Linearity Range (µg/L)	Regression Equation	r ²	LOD (µg/L)	LOQ (µg/L)
ZEN	317.1	175.1 ^a	23	C ₁₁ H ₇ O ₃ -	0.1–100	Y = 2222.2914X -	0.997	0.03	0.1
	[M-H]-	131.1	29	C ₉ H ₇ O-		107.3044			
α-ZEL	319.1	160.1 ^a	33	C ₉ H ₄ O ₃ -	0.1–100	Y = 1526.5935X -	0.999	0.03	0.1
	[M-H]-	188.1	18	C ₉ H ₆ O ₃ -		79.9045			
β-ZEL	319.1	160.1 ^a	33	C ₉ H ₄ O ₃ -	0.1–100	Y = 1721.8353X -	0.998	0.03	0.1
	[M-H]-	188.1	18	C ₉ H ₆ O ₃ -		98.3354			
ZEN-14G	479.1	317.1 ^a	16	C ₁₈ H ₂₁ O ₅ -	0.03–100	Y = 2736.8353X -	0.998	0.01	0.03
	[M-H]-	175.1	40	C ₁₀ H ₇ O ₃ -		48.8494			
α-ZEL-14G	481.2	319.1 ^a	15	C ₁₈ H ₂₃ O ₅ -	0.03–100	Y = 3126.4545X -	0.992	0.01	0.03
	[M-H]-	275.1	34	C ₁₇ H ₂₃ O ₃ -		63.6905			
β-ZEL-14G	481.2	319.1 ^a	15	C ₁₈ H ₂₃ O ₅ -	0.1–100	Y = 2295.981X -	0.999	0.03	0.1
	[M-H]-	275.1	34	C ₁₇ H ₂₃ O ₃ -		122.075			

Where, ^a means quantitation ion; CE stands for collision energy; r², correlation coefficient; LOD, limit of detection; LOQ, limit of quantification (S/N > 10), respectively.

Table S2. Integrated results of analytical method validation.

Compound	Low Spiked Level (LOQ)			Medium Spiked Level (5 LOQ)			High Spiked Level (10 LOQ)		
	R _{ave} (%)	RSD	RSD	R _{ave} (%)	RSD	RSD	R _{ave} (%)	RSD	RSD
		Intra-Day (%)	Inter-Day (%)		Intra-Day (%)	Inter-Day (%)		Intra-Day (%)	Inter-Day (%)
ZEN	81.2	8.3	9.7	85.6	9.0	10.8	83.9	8.9	10.3
α -ZEL	89.3	9.8	11.3	83.5	8.9	9.7	90.4	9.5	10.6
β -ZEL	92.1	10.6	13.2	88.1	9.6	11.4	86.9	9.2	11.6
ZEN-14G	90.4	12.6	14.8	92.4	13.9	14.9	89.6	12.1	13.5
α -ZEL-14G	89.9	11.2	12.9	90.1	13.2	12.9	85.8	13.8	12.8
β -ZEL-14G	86.5	10.1	11.7	81.7	12.0	10.4	85.7	11.9	13.6

Where R_{ave} represents average recovery; RSD, relative standard deviation.