

Table S1. Mass spectra information of benzoxazinoids.

Compound	RT(min)	Ionization	Precursor (<i>m/z</i>)	Neutral Loss fragment(Da)	MS ² Ions <i>m/z</i> (relative intensity)
DHBOA-Glc	5.80	[M+FA-H] ⁻ [M-H] ⁻	388 342	FA (46)	342 (100)
				Glc (162)	180 (100)
				Glc + H ₂ O (180)	162 (6)
				Glc + CO (190)	152 (6)
HBOA-Glc	7.04	[M-H] ⁻	326	Glc (162)	164 (100)
				Glc + CO (190)	136 (6)
				Glc + 2CO (218)	108 (6)
HMBOA-Glc	7.56	[M-H] ⁻	356	Glc (162)	194 (100)
				Glc + CO (190)	166 (5)
				Glc + 2CO (218)	138 (5)
DIMBOA-Glc	7.78	[M+FA-H] ⁻ [M-H] ⁻	418 372	FA (46)	372 (100)
				Glc (162)	210 (27)
				Glc + H ₂ O (180)	192 (18)
				Glc + H ₂ O + CO (208)	164 (100)
				Glc + H ₂ O + CO + CH ₃ (223)	149 (95)
HDMBOA-Glc	9.29	[M+FA-H] ⁻	432	OCH ₃ (31)	401 (13)
				OCH ₃ + FA - H (76)	356 (100)
				Glc + H ₂ O + CO (208)	224 (10)
				Glc + OCH ₃ + FA-H (238)	194 (21)
				Glc + OCH ₃ + CH ₂ O + FA - H (268)	164 (20)
				Glc + OCH ₃ + CH ₂ O + CH ₃ + FA - H (283)	149 (10)
DIMBOA	9.64	[M+FA-H] ⁻ [M-H] ⁻	256 210	FA (46)	210 (100)
				H ₂ O + CO (46)	164 (100)
				H ₂ O + CO + CH ₃ (61)	149 (45)

Note: RT, Retention Time; FA, formic acid; [M + FA - H]⁻, FA adduct; [M - H]⁻, deprotonated ion; Glc, glucoside.