

Table S1. Biotransformation of FBZ in soybean – main peaks detected by UHPLC-MS/MS. Retention time, theoretical molecular weight, molecular formula and selected SRM transitions.

t_R [min]	Theoretical m/z Values of $[M+H]^+$ ions	Elemental Composition	Description of metabolite formation		Product Ions of $[M+H]^+$, m/z	Metabolite Designation
			Phase I	Phase II		
2.631	478.1278	C ₂₁ H ₂₃ N ₃ O ₈ S	2*(+O), hydrolysis	Glycosidation, O-acetylation	258, 133	M1
2.842	478.1278	C ₂₁ H ₂₃ N ₃ O ₈ S	2*(+O), hydrolysis	Glycosidation, O-acetylation	258, 133	M2
3.090	478.1278	C ₂₁ H ₂₃ N ₃ O ₈ S	2*(+O), hydrolysis	Glycosidation, O-acetylation	258, 133	M3
3.504	478.1278	C ₂₁ H ₂₃ N ₃ O ₈ S	2*(+O), hydrolysis	Glycosidation, O-acetylation	258, 133	M4
3.942	478.1278	C ₂₁ H ₂₃ N ₃ O ₈ S	+O	N-glycosidation	316, 284, 191	M5
4.031	478.1278	C ₂₁ H ₂₃ N ₃ O ₈ S	2*(+O), hydrolysis	Glycosidation, O-acetylation	258, 133	M6
5.202	316.075	C ₁₅ H ₁₃ N ₃ O ₃ S	Hydroxylation	-	266, 207	M7
6.086	462.1329	C ₂₁ H ₂₃ N ₃ O ₇ S	-	N-glycosidation	300	M8
6.492	462.1329	C ₂₁ H ₂₃ N ₃ O ₇ S	+O, hydrolysis	Glycosidation, O-acetylation	242	M9
6.567	462.1329	C ₂₁ H ₂₃ N ₃ O ₇ S	-	N-glycosidation	300	M10
6.683	462.1329	C ₂₁ H ₂₃ N ₃ O ₇ S	+O, hydrolysis	Glycosidation, O-acetylation	242	M11
6.891	462.1329	C ₂₁ H ₂₃ N ₃ O ₇ S	+O, hydrolysis	Glycosidation, O-acetylation	242	M12
6.851	462.1329	C ₂₁ H ₂₃ N ₃ O ₇ S	-	N-glycosidation	300, 268	M13
7.256	462.1329	C ₂₁ H ₂₃ N ₃ O ₇ S	+O, hydrolysis	Glycosidation, O-acetylation	242	M14
7.605	462.1329	C ₂₁ H ₂₃ N ₃ O ₇ S	-	N-glycosidation	300, 268	M15
8.08	462.1329	C ₂₁ H ₂₃ N ₃ O ₇ S	-	N-glycosidation	300, 268	M16
9.61	300.0801	C ₁₅ H ₁₃ N ₃ O ₂ S	-	-	268, 159, 131	FBZ