

Table S1. CID product ions of the $[\text{Co}^{2+}(\text{FG} - \text{H})(\text{Aux})_2]^+$ complex of 7-hydroxyflavanone. All minor fragment ions are listed in order of decreasing m/z .

UGT enzyme	CID base peak	other minor fragment ions	assignment
1A1	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide
1A3	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide
1A4	NA	NA	NA
1A6	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide
1A7	-GlcA		7-O-glucuronide
1A8	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide
1A9	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide
1A10	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide

Table S2. CID product ions of the $[\text{Co}^{2+}(\text{FG} - \text{H})(\text{Aux})_2]^+$ complex of 3'-hydroxyflavanone. All minor fragment ions are listed in order of decreasing m/z .

UGT enzyme	CID base peak	other minor fragment ions ^a	assignment
1A1	-Aux	-GlcA, -Agl, -(Agl+Aux)	3'-O-glucuronide
1A3	-Aux	-(Agl+Aux)	3'-O-glucuronide
1A4	NA	NA	NA
1A6	-Aux	-Agl, -(GlcA+Aux), -(Agl+Aux)	3'-O-glucuronide
1A7	-Aux	-GlcA, -(GlcA+Aux), -(Agl+Aux)	3'-O-glucuronide
1A8	-Aux	-(Agl+Aux)	3'-O-glucuronide
1A9	-Aux	-GlcA, -(GlcA+Aux), -(Agl+Aux)	3'-O-glucuronide
1A10	-Aux	-GlcA, -Agl, -(Agl+Aux)	3'-O-glucuronide

^a Variation in fragment ions was noted between some UGT1A reactions due to low S/N for spectra of glucuronides present in low or trace concentrations.

Table S3. CID product ions of the $[\text{Co}^{2+}(\text{FG} - \text{H})(\text{Aux})_2]^+$ complex of 4'-hydroxyflavanone. All minor fragment ions are listed in order of decreasing m/z .

UGT enzyme	CID base peak(s)^	other minor fragment ions ^a	assignment
1A1	-GlcA	-Aux, -Agl, -(GlcA+Aux), -(Agl+Aux)	4'-O-glucuronide
1A3	-GlcA, -(Agl+Aux)	-Aux, -Agl, -(GlcA+Aux)	4'-O-glucuronide
1A4	NA	NA	NA
1A6	-(Agl+Aux)	-GlcA, -Aux, -Agl, -(GlcA+Aux)	4'-O-glucuronide
1A7	NA	NA	NA
1A8	-GlcA	-Aux, -Agl, -(GlcA+Aux), -(Agl+Aux)	4'-O-glucuronide
1A9	NA	NA	NA
1A10	-GlcA, -(Agl+Aux)	-Aux, -Agl, -(GlcA+Aux)	4'-O-glucuronide

^a Variation in fragment ions was noted between some UGT1A reactions due to low S/N for spectra of glucuronides present in low or trace concentrations.

Table S4. CID product ions of the $[\text{Co}^{2+}(\text{FG} - \text{H})(\text{Aux})_2]^+$ complex of 2'-hydroxychalcone. All minor fragment ions are listed in order of decreasing m/z .

UGT enzyme	CID base peak	other minor fragment ions ^a	assignment
1A1	-(GlcA + Aux)		2'-O-glucuronide
1A3	-(GlcA + Aux)	-Aux	2'-O-glucuronide
1A4	NA	NA	NA
1A6	-(GlcA + Aux)		2'-O-glucuronide
1A7	-(GlcA + Aux)		2'-O-glucuronide
1A8	-(GlcA + Aux)	-Aux	2'-O-glucuronide
1A9	-(GlcA + Aux)		2'-O-glucuronide
1A10	-(GlcA + Aux)	-Aux	2'-O-glucuronide

^a Variation in fragment ions was noted between some UGT1A reactions due to low S/N for spectra of glucuronides present in low or trace concentrations.

Table S5. CID product ions of the $[\text{Co}^{2+}(\text{FG} - \text{H})(\text{Aux})_2]^+$ complex of 2',4'-dihydroxychalcone. All minor fragment ions are listed in order of decreasing m/z .

UGT enzyme	CID base peak	other minor fragment ions ^a	assignment
1A1	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide (flavanone)
	-(GlcA + Aux)	-GlcA	2'-O-glucuronide
	-Aux	-GlcA, -(GlcA+Aux)	4'-O-glucuronide
1A3	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide (flavanone)
	-(GlcA + Aux)	-GlcA, -Agl, (2Aux+Co)	2'-O-glucuronide
	-Aux	-GlcA, -(GlcA+Aux), -(Agl+Aux)	4'-O-glucuronide
1A4	NA	NA	NA
1A6	-(GlcA + Aux)	-GlcA	2'-O-glucuronide
	-Aux	-GlcA, -(GlcA+Aux), -(Agl+Aux)	4'-O-glucuronide
1A7	-GlcA	-H ₂ O, -Agl fragment, -Aux, -(Agl+Aux)	7-O-glucuronide (flavanone)
	-(GlcA + Aux)		2'-O-glucuronide
	-Aux	-GlcA, -(GlcA+Aux), -(Agl+Aux)	4'-O-glucuronide
1A8	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide (flavanone)
	-(GlcA + Aux)		2'-O-glucuronide
	-Aux	-GlcA, -(GlcA+Aux), -(Agl+Aux)	4'-O-glucuronide
1A9	-GlcA	-Agl, -(GlcA+Aux), -(Agl+Aux)	7-O-glucuronide (flavanone)
	-(GlcA + Aux)	-GlcA	2'-O-glucuronide
	-Aux	-GlcA, -(GlcA+Aux)	4'-O-glucuronide
1A10	-GlcA		7-O-glucuronide (flavanone)
	-Aux	-GlcA, -(GlcA+Aux)	4'-O-glucuronide

^a Variation in fragment ions was noted between some UGT1A reactions due to low S/N for spectra of glucuronides present in low or trace concentrations.

Table S6. CID product ions of the $[\text{Co}^{2+}(\text{FG} - \text{H})(\text{Aux})_2]^+$ complex of 3,2'-dihydroxychalcone. All minor fragment ions are listed in order of decreasing m/z .

UGT enzyme	CID base peak	other minor fragment ions ^a	assignment
1A1	-Aux	-GlcA, -Agl, -(GlcA+Aux), -(Agl+Aux)	3'-O-glucuronide (flavanone)
	-Aux	-(GlcA+Aux)	3-O-glucuronide
1A3	-Aux	-(GlcA+Aux), -(Agl+Aux)	3'-O-glucuronide (flavanone)
	-Aux	-(GlcA+Aux)	3-O-glucuronide
1A4	NA	NA	NA
1A6	-Aux	-GlcA, -(GlcA+Aux), -(Agl+Aux)	2'-O-glucuronide ^b
1A7	-Aux	-(GlcA+Aux), -(Agl+Aux)	3'-O-glucuronide (flavanone)
	-Aux	-(Agl+Aux)	3-O-glucuronide
1A8	-Aux	-GlcA, -Agl, -(GlcA+Aux), -(Agl+Aux)	2'-O-glucuronide
	-Aux	-(2Aux-GlcA), (GlcA+Aux+Co)	3'-O-glucuronide (flavanone)
	-Aux	-Agl, -(GlcA+Aux), -(Agl+Aux)	3-O-glucuronide
1A9	-(GlcA+Aux)	-GlcA, -Aux, -(Agl+Aux)	2'-O-glucuronide
	-Aux	-(Agl+Aux)	3'-O-glucuronide (flavanone)
	-Aux	-(GlcA+Aux)	3-O-glucuronide
1A10	-Aux	-GlcA, -Agl, -(GlcA+Aux), -(Agl+Aux)	3'-O-glucuronide (flavanone)
	-Aux	-(GlcA+Aux), -(Agl+Aux)	3-O-glucuronide

^a Variation in fragment ions was noted between some UGT1A reactions due to low S/N for spectra of glucuronides present in low or trace concentrations. ^b Present in trace amounts; may be 2'-O-glucuronide according to retention time or 3'-O-glucuronide (flavanone) according to CID fragmentation pattern.

Table S7. CID product ions of the $[\text{Co}^{2+}(\text{FG} - \text{H})(\text{Aux})_2]^+$ complex of 4,2'-dihydroxychalcone. All minor fragment ions are listed in order of decreasing m/z .

UGT enzyme	CID base peak	other minor fragment ions ^a	assignment
1A1	-GlcA	-Aux, -Agl, -(GlcA+Aux), -(Agl+Aux)	4'-O-glucuronide (flavanone)
	-(GlcA+Aux)	-GlcA, -Aux	2'-O-glucuronide
	-Aux	-(GlcA+Aux)	4-O-glucuronide
1A3	-GlcA	-Aux, -Agl, -(GlcA+Aux), -(GlcA+Agl), -(Agl+Aux)	4'-O-glucuronide (flavanone)
	-(GlcA+Aux)	-GlcA, -Aux, -Agl, -(Agl+Aux)	2'-O-glucuronide
	-Aux	-(GlcA+Aux)	4-O-glucuronide
1A4	NA	NA	NA
1A6	-GlcA	-Aux, -Agl, -(GlcA+Aux), -(GlcA+Agl), -(Agl+Aux)	4'-O-glucuronide (flavanone)
	-(GlcA+Aux)	-Aux, -GlcA	2'-O-glucuronide
	-Aux		4-O-glucuronide
1A7*	-GlcA	-(GlcA+Agl)	4'-O-glucuronide (flavanone)
1A8*	-(GlcA+Aux)	-Aux, -GlcA, -(Agl+Aux)	2'-O-glucuronide
1A9*	-(GlcA+Aux)	-GlcA	2'-O-glucuronide
	853 m/z	-(GlcA+Aux), -Aux	4-O-glucuronide
1A10	-(Agl+Aux)	-GlcA, -Agl, -(GlcA+Aux), -Aux	4'-O-glucuronide (flavanone) ^b
	-Aux	-(GlcA+Aux)	4-O-glucuronide

^a Variation in fragment ions was noted between some UGT1A reactions due to low S/N for spectra of glucuronides present in low or trace concentrations. ^b Present in trace amounts; may be 4'-O-glucuronide (flavanone) or 2'-O-glucuronide.

Table S8. CID product ions of the $[\text{Co}^{2+}(\text{FG} - \text{H})(\text{Aux})]^+$ complex of alpinetin. All minor fragment ions are listed in order of decreasing m/z .

UGT enzyme	CID base peak	other minor fragment ions ^a	assignment
1A1	-Agl	-GlcA	7-O-glucuronide-5-methoxyflavanone
1A3	-Agl	-GlcA, -Agl fragment, -(GlcA+Aux)	7-O-glucuronide-5-methoxyflavanone
1A4	NA	NA	NA
1A6	NA	NA	NA
1A7	NA	NA	NA
1A8	-Agl	-GlcA, -Agl fragment, -(GlcA+Aux)	7-O-glucuronide-5-methoxyflavanone
1A9	-Agl	-GlcA, -(GlcA+Aux)	7-O-glucuronide-5-methoxyflavanone
1A10	-Agl	-GlcA	7-O-glucuronide-5-methoxyflavanone

^a Variation in fragment ions was noted between some UGT1A reactions due to low S/N for spectra of glucuronides present in low or trace concentrations.

Table S9. CID product ions of the $[\text{Co}^{2+}(\text{FG} - \text{H})(\text{Aux})]^+$ complex of cardamonin. All minor fragment ions are listed in order of decreasing m/z .

UGT enzyme	CID base peak	other minor fragment ions ^a	assignment
1A1	-Agl	-Agl fragment, -GlcA	7-O-glucuronide-5-methoxyflavanone
	-GlcA		2'-O-glucuronide
	-GlcA		4'-O-glucuronide
			DG
1A3	-Agl	-Agl fragment, -GlcA	7-O-glucuronide-5-methoxyflavanone
	-GlcA		4'-O-glucuronide
1A4	NA	NA	NA
1A6	-GlcA		2'-O-glucuronide
	657 m/z	-Agl fragment, -GlcA, -Aux	4'-O-glucuronide
1A7	-Agl	-GlcA, -(GlcA+Aux), -(GlcA+Aux+CO ₂)	7-O-glucuronide-5-methoxyflavanone
	-GlcA		2'-O-glucuronide
	-GlcA		4'-O-glucuronide
1A8	-Agl	-GlcA, -(GlcA+Aux)	7-O-glucuronide-5-methoxyflavanone
	-GlcA		4'-O-glucuronide
1A9	-Agl	-GlcA, -(GlcA+Aux), -(GlcA+Aux+CO ₂)	7-O-glucuronide-5-methoxyflavanone
	-GlcA		2'-O-glucuronide
	-GlcA		4'-O-glucuronide
1A10	ND	ND	ND
	-GlcA		4'-O-glucuronide

^a Variation in fragment ions was noted between some UGT1A reactions due to low S/N for spectra of glucuronides present in low or trace concentrations.