

High-Throughput Identification of Organic Compounds from *Polygoni Multiflori Radix Praeparata* (*Zhiheshouwu*) by UHPLC-Q-Exactive Orbitrap-MS

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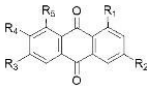
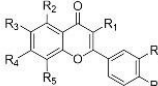

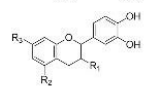
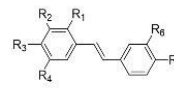
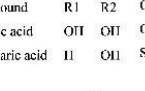
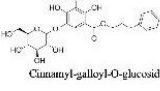
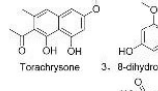
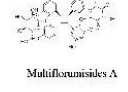
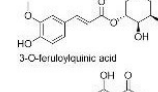
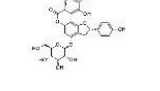
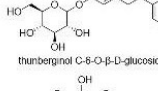
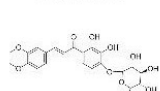
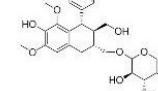
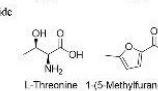
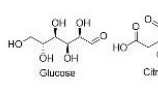
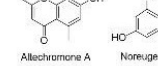
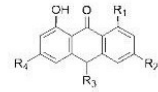
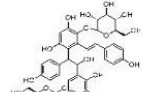
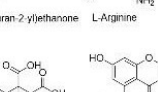
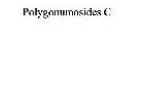
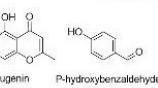
																		
Compound	R1	R2	R3	R4	R5	Compound	R1	R2	R3	R4	R5	R6	R7					
Emodin-8-O-(6'-O-acetyl)-β-D-glucoside	OH	CH3	OH	H	Glc-Ace	Cirsimarin	H	OH	OCH3	OCH3	H	Glc	H					
Chrysophanol	OH	CH3	H	H	OH	Liquiritigenin-glucoside-xy/ara	H	H	H	Xyl	H	Glc	H					
Emodin-O-glucoside-gallate	Gallate	CH3	OH	H	Glc	Hesperetin-7-O-glucoside	H	OH	H	Glc	H	OCH3	OH					
6-Carboxyl emodin	OH	CH2COOH	OH	H	OH	Epimedium	H	OH	H	OH	CH3	OH	H					
Physcion-8-O-β-D-glucoside	Glc	OCH3	CH3	H	OH	Kaempferol-3-β-D-glucoside	Glc	OH	H	OH	H	OH	H					
Physcion	OH	OCH3	CH3	H	OH	Quercetin	OH	OH	H	OH	H	OH	OH					
Citronosin	OH	CH2OH	OH	H	OH	Kaempferol	OH	OH	H	OH	H	OH	H					
Quercetin	OH	CH2OH	OH	H	OCH3	Kaempferol-O-hexose-rhamnose	Glc	OH	H	Rha	H	OH	H					
Hydroxyl-rhein	OH	COOH	OH	H	OH	Dihydroquercetin	OH	OH	H	OH	H	OH	OH					
Digitolein	OCH3	OH	CH2OH	H	OH													
Emodin-3-ethyl ether	OH	OCH2CH3	CH3	H	OH	Compound	R1	R2	R3	R4	R5	Compound	R1	R2	R3			
2-acetylmordin	OH	OH	CH3	COCH3	OH	Gallate acid	H	OH	OH	OH	H	Catechin	OH	OH	OH			
Emodin	OH	CH3	OH	H	OH	Gallate acid-O-glucoside	H	OH	OH	Glc	H	Acetyl-picatechin-O-glucoside	OH	Glc	Acc			
Emodin-8-O-β-D-glucoside	OH	CH3	OH	H	Glc	Dihydroxy-benzoic acid	OH	H	H	H	OH	Epicatechin-O-gallate	Gal	OH	OH			
Physcion-8-O-(6'-O-malonyl)-hexose	Glc-Mal	OCH3	CH3	H	OH	Vanillic acid	H	OCH3	OH	H	H	Protocatechuic acid-O-glucoside	OH	OH	OH			
Citronosin-O-glucoside	OH	CH2OH	OH	H	Glc	Protocatechuic acid-O-glucoside	H	Glc	OH	H	H	Veratric acid	H	OCH3	OCH3			
						Veratric acid	H	OCH3	OCH3	H	H	Compound	R1	R2	Compound	R		
Compound	R1	R2	R3	R4	R5	R6	3-Hydroxybenzoic acid	H	OH	H	H	H	Caffeic acid	OH	OH	Gallate-glycerol	Gly	
3,4,5,4'-tetrahydroxystilbene	H	OH	OH	OH	OH	H	2-Methyl gallate	CH3	OH	OH	OH	OH	Coumaric acid	H	OH	Syringic acid	OCH3	
Rhapontin	H	OH	H	Glc	OCH3	OH	Syringic acid	H	OCH3	OH	OCH3	H						
Tetrahydroxystilbene-O-di-glucoside	Glc	OH	H	Glc	OH	H												
Resveratrol	H	OH	H	OH	OH	H												
(Z)-2, 3, 5, 4'-	Glc	OH	H	OH	OH	H												
Tetrahydroxystilbene-2-O-β-D-glucoside	Mal	OH	H	Glc	OH	H												
2,3,5,4'-Tetrahydroxystilbene-O-(malonyl)-β-D-glucoside	Glc	OH	H	Gal	OH	H												
Tetrahydroxystilbene-O-(galloyl)-glucoside	H	OH	H	Gal	OH	H												
Piceatannol-3-O-β-D-(6'-O-galloyl)-glucoside	H	O-Glc	H	OH	OH	H												
Tetrahydroxystilbene-O-(caffeoyl)-glucoside	Glc	OH	H	Caf	OH	H												
Polydatin	H	O-Glc	H	OH	OH	H												
Isorhapontigenin	H	OH	H	OH	OH	H												
2,3,5,4'-tetrahydroxystilbene-2-O-β-D-(2"-O-coumaroyl)-glucoside	Glc	OH	H	OH	OH	H												
2,3,5,4'-tetrahydroxystilbene-2-O-(2"-O-acetyl)-β-D-glucoside	Cou	OH	H	OH	OH	H												
Tetrahydroxystilbene-2-(feruloyl)-glucoside	Glc	OH	H	Fer	OH	H												
																		
Compound	R1	R2	R3	R4														
Rumicapsoside D	OH	OH	Glc	CH2OH														
Di-Emodin anthrone-Di-glucoside	Glc	H	H	EA-Glc														
Chrysophanol anthrone	H	H	H	CH3														
Emodin anthrone	OH	OH	H	CH3														

Figure S1. Chemical structures of compounds identified in PMRP. Glc: glucoside; Mal: malonyl; Ace: acetyl; EA: Emodin anthrone; Gal: galloyl; Cou: coumaroyl; Fer: feruloyl; Caf: caffeoyl; Rha: rhamnose; Xyl: xylose; Gly: glycerol.