

**Table. S3. The detail data for VIP value.**

	No.	Compounds	VIP	Type
LF-OMTMS-D vs MF-OMTMS-D	1	1-O-Galloyl-2-O-Cinnamoyl-β-D-glucose	1.56	down
	2	4-Nitrophenol	1.55	down
	3	Sinapic acid	1.55	up
	4	Syringaldehyde; 4-Hydroxy-3,5-Dimethoxybenzaldehyde	1.55	down
	5	Methyl gallate	1.55	up
	6	4-O-Methylgallie Acid	1.54	up
	7	Sideretin (5,7,8-Trihydroxy-6-methoxycoumarin)	1.54	up
	8	Kaempferol-7-O-glucoside*	1.53	up
	9	Furanofructosyl-α-D-(6-mustard acyl)glucoside*	1.53	up
	10	6'-O-Sinapoylsucrose*	1.53	up
	11	Quercetin-4'-O-glucoside (Spiraeoside)*	1.52	up
	12	Chrysoeriol-5-O-glucoside	1.51	up
	13	1-O-Sinapoyl-β-D-glucose	1.51	up
	14	Hesperetin-5-O-glucoside	1.49	up
	15	Kaempferol-3-O-galactoside (Trifolin)*	1.49	up
	16	Quercetin-3-O-glucoside (Isoquercitrin)*	1.49	up
	17	3-(3-Hydroxyphenyl)-3-hydroxypropanoic acid	1.48	down
	18	Kaempferol-3-O-rhamnoside (Afzelin)(Kaempferin)*	1.45	up
	19	3-O-p-Coumaroylshikimic acid	1.45	down
	20	Quercetin-7-O-glucoside*	1.43	up
LF-OMTMS-D vs HF-OMTMS-D	1	Gambirinin A1	1.37	up
	2	Syringaldehyde; 4-Hydroxy-3,5-Dimethoxybenzaldehyde	1.37	down
	3	Protocatechuic Acid Methyl Ester	1.37	up
	4	Glucosyringic acid	1.37	up
	5	Kaempferol-7-O-rhamnoside*	1.37	up
	6	4-Nitrophenol	1.37	down
	7	Sinapic acid	1.36	up
	8	4-O-Methylgallie Acid	1.36	up
	9	Methyl gallate	1.36	up
	10	7-Methoxy-3-[1-(3-pyridyl)methylidene]-4-chromanone	1.36	up
	11	Chrysoeriol-5-O-glucoside	1.36	up
	12	Kaempferol-7-O-glucoside*	1.36	up
	13	Quercetin-7-O-rutinoside*	1.36	up
	14	1-O-Sinapoyl-β-D-glucose	1.36	up
	15	3,4-Methylenedioxy cinnamyl alcohol	1.36	up
	16	Quercetin-4'-O-glucoside (Spiraeoside)*	1.36	up
	17	Syringin	1.35	up
	18	p-Coumaric acid methyl ester	1.35	up
	19	Quercetin-3-O-glucoside (Isoquercitrin)*	1.35	up
	20	Sideretin (5,7,8-Trihydroxy-6-methoxycoumarin)	1.35	up

MF-OMTMS-D vs HF-OMTMS-D

1	Gambirinin A1	1.50	up
2	Gallactophenone	1.50	up
3	1-hydroxy-7-[[2s,3r,4s,5r,6r]-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}xanthen-9-one	1.50	down
4	Syringin	1.49	up
5	1-O-Galloyl-2-O-Cinnamoyl-β-D-glucose	1.49	up
6	7-Methoxy-3-[1-(3-pyridyl)methylidene]-4-chromanone	1.47	up
7	Hydroxyferulic acid glucoside	1.47	up
8	Quercetin-4'-O-glucoside (Spiraeoside)*	1.47	up
9	Quercetin-3-O-glucoside (Isoquercitrin)*	1.46	up
10	Chrysoeriol-5-O-glucoside	1.46	up
11	Hesperetin-5-O-glucoside	1.46	up
12	Quercetin-3-O-arabinoside	1.46	up
13	Kaempferol-7-O-glucoside*	1.46	up
14	Hispidulin-7-O-glucoside(Homoplantaginin)*	1.45	up
15	Kaempferol-7-O-rhamnoside*	1.45	up
16	Apigenin-6-C-arabinoside-8-C-xyloside*	1.44	up
17	Apigenin-6,8-di-C-arabinoside*	1.44	up
18	Kaempferol-3-O-galactoside (Trifolin)*	1.44	up
19	Quercetin-7-O-glucoside*	1.43	up
20	3-O-p-Coumaroylshikimic acid	1.39	down

\* represents the presence of an isomer of the compound.