

Supplementary Table 2 Compound in ZSXBGZ decoction.

Traditional Chinese Medicine	Compound
Fructus Aurantii Immaturus	limonene / dipentene C10H16 3,8-di-C-glucosylapigenin C28H32O16 3,8-di-C-glucosyldiosmetin C27H32O15 syringin eleutheroside B C17H24O9 β -caryophyllene C15H24 caryophellene C15H24 5,7,4'-trimethoxyflavone C18H16O5 nobiletin C21H22O8 nobiletin-3-O- β -glucoside C27H32O14 3-hydroxy-5,6,7,8,3',4'-hexamethoxyflavone-3 β -glucoside / nobiletin-3-O- β -glucoside C27H32O14 lonicerin / lonicrin C27H30O15 2"-O- β -xylosylvitexin C26H28O14 sinensetin / 5,6,7,3',4'-pentamethoxyflavone C20H20O7 5,6,7,8,4'-pentamethoxyflavone / tangeretin C20H20O7 5,7,8,3',4'-pentamethoxyflavone C20H20O7 myrcene C10H16 deacetyl nomilin C26H32O8 deacetyl nomilinic acid C26H34O9 dehydrodiconiferylalcohol-4- β -D-glucoside C26H32O11 6-methoxyaurapten C20H24O4 N-methyltyramine C9H13NO 5,7,3',4'-tetramethoxyflavanone C19H18O6 5,7,8,4'-tetramethoxyflavone C19H18O6 eriocitrin C27H32O15 p-cymol / p-cymene C10H14 linoleic acid C18H32O2 isopimpinellin C13H10O5 isoponcimarin C19H22O5 isolimonic acid C26H32O9 isosakuranetin-7-rutinoside C28H34O14 limonin C26H30O8 synephrine C9H13NO2 γ -terpinene C10H16 α -terpineol-8 β -D-glucopyranoside C16H28O6 coniferin C16H22O8 imperatorin C16H14O4 nomilin C28H34O9

<p>Trichosanthes kirilowii Maxim</p>	<p>nomilinic acid C28H36O10 ichangin C27H34O8 citrusin II C37H44N8O7 citrusin A C26H34O12 citrusin B C27H36O13 narirutin C27H32O14 narirutin / naringenin-7-rutinoside C27H32O14 naringin C27H32O14 naringenin-4'-glucoside-7-rutinoside C33H42O19 poncirin C27H32O12 poncimarin C19H22O5 obaculactone / limonin C25H28O8 evodin C26H28O9 carveol-6 β -glucopyranoside C16H26O7 bergapten C12H8O4 heraclenin C16H14O5 prangenin / heraclenin C16H16O6 prangenin hydrate C16H16O6 obacunone C26H30O7 rhoifolin C27H30O14 7-geranyloxycoumarin C19H22O3 19-hydroxydeacetylnomilinic acid-17- β -D-glucoside C32H46O16 9-hydroxylinalool-9 β -glucopyranoside C16H28O7 aurapten C15H16O4 α -pinene C10H16 β -pinene C9H14O vomifoliol-9-O- β -D-glucopyranoside C19H30O8 neohesperidin C28H34O15 camphene C10H16 hesperidin C28H34O15 hesperidin / hesperetin-7-O-rutinoside C28H34O15 citrusin III C36H53N7O9 citrusin IV C41H55N9O14 citrusin C C16H22O7 aurapten C19H22O3 γ -terpinene C10H16 α -terpineol-8 β -D-glucopyranoside C16H28O6 5,6,7,8,4'-pentamethoxyflavone / tangeretin C20H20O7 5,6,7,8,3',4'-hexamethoxy flavone aspartate / asparagic acid / asparaginic acid / aspartic acid C4H7NO4 glycine C2H5NO2 alanine C3H7NO2</p>
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	methionine C ₅ H ₁₁ NO ₂ S
	cysteine C ₂ SH ₂ O ₆
	serine C ₃ H ₇ NO ₃
	tryptophane C ₁₁ H ₁₂ N ₂ O ₂
	isoleucine C ₆ H ₁₃ NO ₂
	threonine C ₄ H ₉ NO ₃
	glutamic acid C ₅ H ₉ NO ₄
	phenylalanine C ₉ H ₁₁ NO ₂
	histidine C ₆ H ₉ N ₃ O ₂
	leucine C ₆ H ₁₃ NO ₂
	proline C ₅ H ₉ NO ₂
	lysine C ₆ H ₁₄ N ₂ O ₂
	tyrosine C ₉ H ₁₁ NO ₃
	arginine C ₆ H ₁₄ N ₄ O ₂
	valine C ₅ H ₁₁ NO ₂
	Karounidiol 3-benzoate
	Trichosanatine
	Trichosanic acid
	7-Oxoisomultiflorenol
	5 α -Stigmastane-3 β ,6 α -diol
	γ -Aminobutyric acid
	CucurbitacinJ2-O- β -glucopyranoside
	Cyclotricuspidoside A
	Cyclotricuspidoside B
	Cyclotricuspidoside C
	(25R)-Samogenin3-O- β -D-glucopyranosyl(1->2)- β -D-ga...
	(25S)-Samogenin3-O- β -D-glucopyranosyl(1->2)- β -D-ga...
	CucurbitacinK2-O- β -glucopyranoside
	3-Epibryonolol
	3-Epikarounidiol
	Vomifoliol
	7-Oxodihydro karounidiol
	Bryonolic acid
	Karounidiol
	7-Stigmastenol-3-O- β -D-glucoside
	7-Stigmastene-3
	3,29-O-Dibenzoyloxykarounidiol
	Hexadecanoicacid
	11-Methoxynoryangonin
	Khekadaengoside C
Allium	dipropyl disulfide C ₆ H ₁₄ S ₂
Macrostemon	
Bunge	dipropyl trisulfide C ₆ H ₁₄ S ₃

dimethyl disulfide C₂H₆S₂
dimethyl trisulfide C₂H₆S₃
3,5-dimethyl-1,2,4-trithiane C₅H₁₀S₃
3,3-dimethylpentane C₇H₁₆
dimethyl tetrasulfide C₂H₆S₄
2,4-dimethyl thiophene C₆H₈S
1,2-dimethylthioethylene C₄H₈S₂
diallyl disulphide / diallyl disulfide / allyl disulfide C₆H₁₀S₂
1,3-dithiane C₄H₈S₂
succinic acid C₄H₆O₄
daturic acid / heptadecanoic acid / margaric acid C₁₇H₃₄O₂
heptadecenoic acid C₁₇H₃₀
9,12-octadecadienoic acid C₁₈H₃₂O₂
pentadecanoic acid C₁₅H₃₀O₂
hexadecenoic acid C₁₆H₃₀O₂
2,2-bis(methylthio)propane C₅H₁₂S₂
n-propylmethyl trisulfide C₄H₁₀S₃
n-heptane C₇H₁₆
propylisopropyl disulfide C₆H₁₄S₂
3-[(1-methyl ethyl)thiol]-1-propene C₆H₁₂S
21-methyl tricosanoic acid C₂₄H₄₈O₂
4-methyl-1,2,3-trithiane C₄H₈S₃
3-methylhexane C₇H₁₆
methyl propyl disulfide C₄H₁₀S₂
methyl propyl trisulfide C₄H₁₀S₃
methyl(1-propenyl)-disulfide C₄H₈S₂
2-methyl-2-pentenal C₆H₁₀O
5-methyl-1,2,3,4-tetrathiane C₃H₆S₄
methylcyclohexane C₇H₁₄
methyl allyl disulfide C₄H₈S₂
methyl allyl trisulfide C₄H₈S₃
lunularic acid C₁₅H₁₄O₄
N-(p-trans-coumaroyl)tyramine C₁₇H₁₇NO₃
p-coumaric acid C₉H₈O₃
p-coumaric acid / 4-hydroxycinnamic acid C₉H₈O₃
N-(p-cis-coumaroyl)tyramine C₁₇H₁₇NO₃
p-hydroxybenzoic acid C₇H₆O₃
linoleic acid C₁₈H₃₂O₂
isopropylallyl disulfide C₆H₁₂S₂
smilagenin-3-O- β -D-glucopyranosyl(1 → 2)- β -D-galactopyranoside
C₄₀H₆₆O₁₂
β -sitosterol-3-O- β -D-glucopyranoside / daucosterol / strumaroside /
daucosterin C₃₅H₆₀O₆
eleutheroside A C₃₅H₆₀O₆

Mangolia officinalis	alexandrin C35H60O6 N-ferulosyl tyramine C18H19NO4 chinenoside I C46H74O23 prostaglandin A1 C20H32O4 adenosine / adenine nucleoside C10H13N5O4 macrostemonoside A C51H84O23 prostaglandin B1 C20H32O4 macrostemonoside D C53H86O24 macrostemonoside E C57H94O28 macrostemonoside F C45H74O18 n-propylallyl disulfide 3-[(1-methyl ethyl)thiol]-1-propene macrostemonoside B macrostemonoside C Magnolol Honokiol Magnocurarine Obovatol Magnotriol B Magnotriol A N-Acetylxylopine N-Acetylanonaine 1,1'-Dibenzene-6',8',9'-trihydroxy-3-allyl-4-O- β -D... N-Formylanonaine Clovanemagnolol Caryolanemagnolol Eudesobovatol A 1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(omega-hydroxypr... Asimilobine Monoterpenylmagnolol (-)-Anonaine Randaiol Piperitylmagnolol Piperitylhonokiol Magnolignan I Magnolignan H Magnolignan G Magnolignan F Magnolignan E Magnolignan D Magnolignan C Magnolignan B Magnolignan A
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Cassia twig	Magnatriol B Magnaldehyde E Magnaldehyde D Magnaldehyde C Magnaldehyde B 6'-O-Methylhonokiol Isomagnolol Dipiperitylmagnolol Bornul magnolol cinnamyl acetate C ₁₁ H ₁₂ O ₂ benzyl benzoate / phenylmethylbenzoate C ₁₄ H ₁₂ O ₂ coumarin C ₉ H ₆ O ₂ cinnamaldehyde / cinnamic aldehyde C ₉ H ₈ O calamenene C ₁₅ H ₂₂ calamenene C ₁₅ H ₂₂ β-cadinene Anhydrocinnzeylanol 2-Methoxycinnamaldehyde
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