

**Table S2.** Homoisoflavonoid derivatives isolated from Fabaceae family

Plant species	Subjected soluble fraction/plant part	Method of isolation/purification	Name	Reference
<i>Caesalpinia bahamensis</i>	MeOH/R	FC [CH <sub>2</sub> Cl <sub>2</sub> –EtOAc], HPLC [H <sub>2</sub> O (0.1% HCO <sub>2</sub> H)–MeCN (0.1% HCO <sub>2</sub> H)]	metasappanin [syn. 3-(2-hydroxy-4-methoxybenzyl)chromane-4,7-diol]	[92]
<i>Caesalpinia bonduc</i>	EtOH/bark	CC [NHEX–CHCl <sub>3</sub> 100:0 to 0:100; CHCl <sub>3</sub> –MeOH 100:0 to 0:100], CC [CHCl <sub>3</sub> –MeOH 85:15], PTLC [CH <sub>2</sub> Cl <sub>2</sub> –MeOH 75:25]	caesalpinianone	[5]
			6- <i>O</i> -methylcaesalpinianone	
<i>Caesalpinia digyna</i>	MeOH/R	CC [NHEX–EtOAc 65:35 to 60:40]	( <i>Z</i> )-7,8-dihydroxy-3-(4'-methoxybenzyl)chroman-4-one (syn. isointricatinol)	[93]
		CC [NHEX–EtOAc 75:25 to 65:35]	intricatinol	
		HPLC [MeOH–H <sub>2</sub> O 60:40]	( <i>Z</i> )-7-hydroxy-8-methoxy-3-(4'-methoxybenzyl)chroman-4-one	
			8-methoxybonducellin	
		HPLC [MeOH–H <sub>2</sub> O 75:25]	<i>Z</i> -eucomine	
			<i>E</i> -eucomine	
		HPLC [MeOH–H <sub>2</sub> O 70:30]	isobonducellin	
<i>Caesalpinia japonica</i>	CH <sub>2</sub> Cl <sub>2</sub> /heartwood		bonducellin	[94]
		SLH	demethyleucomine	
		PTLC [CHCl <sub>3</sub> –EtOAc 9:1]	3'-deoxy-4- <i>O</i> -methylsappanol (syn. 3,7-dihydroxy-3-(4-hydroxybenzyl)-4-methoxychroman)	
			4- <i>O</i> -methylepisappanol	
		CC	4- <i>O</i> -methylsappanol	
		PTLC [CHCl <sub>3</sub> –EtOAc 7:1]	sappanol	
			episappanol	
<i>Caesalpinia latisiliqua</i>	EtOAc/twig		sappanone A	[95]
		PTLC	sappanone B	
<i>Caesalpinia latisiliqua</i>	EtOAc/twig	HPLC [MeCN–H <sub>2</sub> O 35:65]	(3 <i>S</i> )-dihydrobonducellin 8- <i>O</i> -β-D-glucopyranoside	[95]
<i>Caesalpinia millettii</i>	Me <sub>2</sub> CO/St	SLH [MeOH]	8-methoxyisobonducellin	[96]
			8-methoxybonducellin	
		CC [CHCl <sub>3</sub> –MeOH 10:0 to 1:1], CC [NHEX–CHCl <sub>3</sub> 9:1]	eucomin	

<i>Caesalpinia sappan</i>	EtOAc/heartwood	CC [NHEX–EtOAc 9:1]	bonducellin	[101]
		SLH [MeOH], CC [NHEX–EtOAc 7:3]	intricatinol	
		RP-CC [MeOH–H <sub>2</sub> O 40:60]	sappanone A	
			3'-deoxy-4- <i>O</i> -methylsappanol	
		RP-CC [MeCN–H <sub>2</sub> O 60:40]	3-deoxysappanone B	
			sappanol	
			7,3',4'-trihydroxy-3-benzyl-2 <i>H</i> -chromene	
			episappanol	
		RP-CC [MeCN–H <sub>2</sub> O 70:30]	sappanone B	
			4-(7-hydroxy-2,2-dimethyl-9 $\beta$ <i>H</i> -1,3,5-trioxa-cyclopenta[ $\alpha$ ]naphthalene-3-lymethyl)-benzene-1,2-diol	
		RP-CC [MeOH–H <sub>2</sub> O 80:20]	4- <i>O</i> -methylepisappanol	
		SLH	4- <i>O</i> -methylsappanol	
		HPLC [MeOH–H <sub>2</sub> O 30:70 (0.1% TFA)]	caesalпинiaphenol A	[102]
			3-deoxysappanone B	
			sappanone A	
		HPLC [MeOH–H <sub>2</sub> O 40:60 (0.1% TFA)]	caesalпинiaphenol B	
		HPLC [MeOH–H <sub>2</sub> O 35:65 (0.1% TFA)]	3'-deoxy-4- <i>O</i> -methylepisappanol	
			3'-deoxysappanone A	
		HSCCC [CHCl <sub>3</sub> –MeOH–H <sub>2</sub> O 4:3:2]	3'-deoxysappanol	[103]
			3-deoxysappanone B	
			4- <i>O</i> -methylsappanol	
			brazilin	
		CC [CHCl <sub>3</sub> –MeOH 95:5], CC [CHCl <sub>3</sub> –Me <sub>2</sub> CO 95:5, 92:8, 88:12], SLH [MeOH–H <sub>2</sub> O 70:30]	7,3',4'-trihydroxy-3-benzyl-2 <i>H</i> -chromene	[104]
			4- <i>O</i> -methylsappanol	
			4- <i>O</i> -methylepisappanol	
			3'-deoxy-4- <i>O</i> -methylsappanol	
		CC [CHCl <sub>3</sub> –MeOH 95:5], CC [CHCl <sub>3</sub> –Me <sub>2</sub> CO 9:1, 85:15, 8:2, 7:3], CC [CH <sub>2</sub> Cl <sub>2</sub> –Me <sub>2</sub> CO 92:8, 9:1, 85:15], SLH [MeOH–H <sub>2</sub> O 60:40]	caesalpin J	
			protosappanin A	
		CC [CHCl <sub>3</sub> –MeOH 100:0 to 70:30], CC [CHCl <sub>3</sub> –MeOH 95:5 to 80:20], SLH [CHCl <sub>3</sub> –	3',4-di- <i>O</i> -methylepisappanol (syn. (3 <i>R</i> ,4 <i>R</i> )-3,7-dihydroxy-3-(3'-methoxy-4'-hydroxybenzyl)-4-methoxychroman	
			caesalпинiaphenol F	

		MeOH 65:35], RP-CC [MeOH–H <sub>2</sub> O 60:40], HPLC [MeOH–H <sub>2</sub> O 50:50]		
	MeOH/heartwood	SLH [MeOH], PTLC	7-hydroxy-3-(4'-hydroxybenzylidene)-chroman-4-one 3,7-dihydroxy-3-(4'-hydroxybenzyl)-chroman-4-one 3,4,7-trihydroxy-3-(4'-hydroxybenzyl)-chroman 7-hydroxy-8-methoxy-3-(4'-methoxybenzylidene)-chroman-one 8-methoxybonduallin	[105]
	n.d/heartwood	n.d	4-O-methylsappanol protosappanin A brazilin caeasalpin J	[106]
	n.d	CPC [EtOAc–MeCN–H <sub>2</sub> O 1:1:2]	sappanol brazilin	[107]
<i>Caesalpinia pulcherrima</i>	CHCl <sub>3</sub> –MeOH/AP	PTLC [NHEX–EtOAc 3:10]	[(3E)-3-(1,3-benzodioxol-5-ylmethylene)-2,3-dihydro-7-hydroxy-4H-1-benzopyran-4-one] [(3E)-2,3-dihydro-7-hydroxy-3-[(4-methoxyphenyl)methylene]-4H-1-benzopyran-4-one] (syn. bonducellin)	[108]
		PTLC [NHEX–EtOAc 1:9]	[(3E)-3-(1,3-benzodioxol-5-ylmethylene)-2,3-dihydro-7-methoxy-4H-1-benzopyran-4-one] [(3E)-2,3-dihydro-7-methoxy-3-[(4-methoxy-phenyl)methylene]-4H-1-benzopyran-4-one] (syn. 7-O-methyl bonducellin) (3E)-2,3-dihydro-6,7-dimethoxy-3[(3-hydroxy-4-methoxyphenyl)methylene]-4H-1-benzopyran-4-one	
		PTLC [NHEX–EtOAc 4:10]	[(3E)-2,3-dihydro-3[(3,4-dihydroxyphenyl)methylene]-7-hydroxy-4H-1-benzopyran-4-one] (syn. sappanone A) [(3E)-2,3-dihydro-7-hydroxy-3-[(3-hydroxy-4-methoxyphenyl)-methylene]-4H-1-benzopyran-4-one]	
		CC [NHEX–EtOAc 1.5:10]	[(3E)-2,3-dihydro-3-[(3,4-dimethoxyphenyl)methylene]-7-methoxy-4H-1-benzopyran-4-one]	
		PTLC [NHEX–EtOAc 3.5:10]	[(3E)-2,3-dihydro-3-[(2,4-dimethoxyphenyl)methylene]-7-hydroxy-4H-1-benzopyran-1-one] (syn. 2'-methoxybonducellin)	
	NHEX/WP	CC [NHEX–EtOAc 95:5]	(E)-7-methoxy-3-(4'-methoxybenzylidene)chroman-4-one	[109]
	Me <sub>2</sub> CO/WP	CC [NHEX–EtOAc 75:25]	(Z)-7-hydroxy-3-(4'-methoxybenzylidene)chroman-4-one (syn. isobonducellin)	

		CC [NHEX–EtOAc 70:30]	( <i>E</i> )-7-hydroxy-3-(4'-methoxybenzylidene)chroman-4-one (syn. bonducellin)	[110]
		CC [NHEX–EtOAc 60:40]	( <i>E</i> )-7-hydroxy-3-(2',4'-dimethoxybenzylidene)chroman-4-one	
			( <i>E</i> )-7-hydroxy-3-(3',4',5'-trimethoxybenzylidene)chroman-4-one	
	Me <sub>2</sub> CO/AP	CC [NHEX–EtOAc 60:40, 65:35]	isobonducellin	
		CC [NHEX–EtOAc 60:40]	bonducellin	
		CC [NHEX–EtOAc 60:40]	isobonducellin	
	CHCl <sub>3</sub> /St		bonducellin	[110–112]
		CC [CHCl <sub>3</sub> –EtOAc], recryst. [CHCl <sub>3</sub> , MeOH]	bonducellin	
		CC [CHCl <sub>3</sub> –EtOAc], PTLC [CHCl <sub>3</sub> –EtOAc 3:1]	8-methoxybonducellin	
	<i>n</i> -BuOH/cork tissue	CC [NHEX–Me <sub>2</sub> CO 5:1 to 1:1], HPLC [MeCN–H <sub>2</sub> O 37:63], PTLC [CHCl <sub>3</sub> –Me <sub>2</sub> CO 12:1]	dihydrobonducellin	[114]
			2'-methoxydihydrobonducellin	
			2'-methoxybonducellin	
			isobonducellin	
		CC [NHEX–Me <sub>2</sub> CO 5:1 to 1:1], recryst.	bonducellin	
<i>Crotalaria pallida</i> Ait	CH <sub>2</sub> Cl <sub>2</sub> /Se	SLH [CH <sub>2</sub> Cl <sub>2</sub> –MeOH 2:1], HPLC [MeOH–H <sub>2</sub> O 58:42]	cropalliflavone A	[115]
			cropalliflavone B	
<i>Heamatoxylon campechianum</i>	EtOAc/St	HPLC [MeCN–H <sub>2</sub> O 10:90 to 35:65]	hematoxylol	[14]
			hematoxylone	
			isohematoxylin	
			epihematoxylol	
			sappanone B	
		HPLC [MeCN–H <sub>2</sub> O 10:90 to 30:70]	4- <i>O</i> -methylepihematoxylol	
			hematoxylene	
			4- <i>O</i> -methylsappanol	
			hematoxin	
			4- <i>O</i> -methylhematoxylol	
	CH <sub>2</sub> Cl <sub>2</sub> /St	SLH [MeOH]	epihematoxin	
			sappanol	
			3'-deoxy- <i>O</i> -methylsappanol	
			3'-deoxy-sappanone A	
		CC [CHCl <sub>3</sub> –MeOH 40:1 to 6:1]	3'-deoxy-sappanone A	
		SLH [CHCl <sub>3</sub> –MeOH 1:1]	sappanene	

		CC [Me <sub>2</sub> CO–PE 3:1 to 1:1]	sappanone A	
		CC [CHCl <sub>3</sub> –MeOH 100:1 to 50:1]	isoliquiritigenin	
			bonducellin	
		CC [Me <sub>2</sub> CO–PE 6:1 to 3:1]	( <i>E</i> )-eucomin	
		CC [Me <sub>2</sub> CO–PE 3:1 to 1:1]	butein	
			sappanchalcone	
		CC [CHCl <sub>3</sub> –MeOH 100:1 to 40:1]	3'-deoxy-sappanchalcone	
	EtOAc/heartwood	RP-CC [MeOH–H <sub>2</sub> O 10:90 to 50:50], HPLC [MeCN–H <sub>2</sub> O 10:90 to 30:70]	hematoxylol B	[116]
			epihematoxylol B	
			caesalpin J	
		HPLC [MeCN–H <sub>2</sub> O 10:90 to 35:65]	1'- <i>O</i> -methylhematoxylol B	
	MeOH/heartwood	CC [CHCl <sub>3</sub> –MeOH 20:1 to 3:1], SLH [CHCl <sub>3</sub> –MeOH 1:1]	1'- <i>O</i> -methylepihematoxylol B	[117]
			hematoxylin	
			hematoxylol A	
		CC [CH <sub>2</sub> Cl <sub>2</sub> –Me <sub>2</sub> CO]	4- <i>O</i> -methylhematoxylol	
<i>Hoffmanosseggia intricata</i>	CHCl <sub>3</sub> /R	CC [CH <sub>2</sub> Cl <sub>2</sub> –MeOH 95:5, 98:2], recryst.	hematoxin	[12]
			intricatin (syn. 7,4'-dimethoxy-8-hydroxyhomoisoflavone)	
<i>Pterocarpus marsupium</i>	Et <sub>2</sub> O/heartwood	CC [Bz; Bz–EtOAc; Bz–EtOAc 7:3]	intricatinol (syn. 4'-methoxy-7,8-dihydroxyhomoisoflavone)	
			pteromarsupone (syn. 6-hydroxy-7- <i>O</i> -methyl-3-(3-hydroxy-4- <i>O</i> -methylbenzyl)chroman-4-one)	[118]
<i>Stuhlmannia moavi</i>	EtOAc/R	SLH [CH <sub>2</sub> Cl <sub>2</sub> –MeOH 1:1], recryst.		[119]
			bonducellin	

AP: aerial part; Bz: benzene; CC: column chromatography; CHCl<sub>3</sub>: chloroform; CH<sub>2</sub>Cl<sub>2</sub>: dichloromethane; CPC: centrifugal partition chromatography; EtOAc: ethyl acetate; EtOH: ethanol; H<sub>2</sub>O: water; HPLC: high-performance liquid chromatography; HSCCC: high-speed counter-current chromatography; L: leaf; MeOH: methanol; Me<sub>2</sub>CO: acetone; MeCN: acetonitrile; *n*-BuOH: butanol; n.d: not determined; NHEx: *n*-hexane; PE: petroleum ether; PTLC: preparative-thin layer chromatography; R: root; recryst.: recrystallization; RP-CC: reverse-phase column chromatography; Se: seed; SLH: Sephadex® LH-20; St: stem; TFA: trifluoroacetic acid; WP: whole part