

Supplementary Materials

Recent advances in Cassane Diterpenoids: Structural Diversity and Biological Activities

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Table S1: List of new usual cassane diterpenoids reported from 2019 to 2025.

Compound Name	M. Wt.	Mol. Formula	Plant, Family, Part used, and Location	Extract/Fraction	Ref.
Taepeenin WA (1)	288	C ₂₀ H ₃₂ O	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	EtOH/Petroleum ether	1
Cassan-13,15-dien-3-oxo-17-oic acid (2)	316	C ₂₀ H ₂₈ O ₃	<i>Erythrophleum suaveolens</i> (Guill. et Perr.) Brenan, (Fabaceae), root barks, Toumodi (Cote d'Ivoire)	MeOH/CH ₂ Cl ₂	2
Cassan-15-en-[7,17]- γ -lactone (3)	300	C ₂₀ H ₂₈ O ₂	<i>Erythrophleum suaveolens</i> (Guill. et Perr.) Brenan, (Fabaceae), root barks, Toumodi (Cote d'Ivoire)	MeOH/CH ₂ Cl ₂	2
3-Deacetyldecapetpene B (4)	362	C ₂₂ H ₃₄ O ₄	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	3
Phanginin JF (5)	302	C ₂₀ H ₃₀ O ₂	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, Qinzhou, Guangxi, China	95% EtOH/CHCl ₃	4
Caesamin E (6)	436	C ₂₃ H ₃₂ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Anguo market of material medica, Hebei, China	Acetone	5
Caesalbonducin N (7)	536	C ₂₈ H ₄₀ O ₁₀	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOAc	6
16-O-Ethyl caesalpin A (8)	476	C ₂₆ H ₃₆ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	7
16-O-Ethyl caesalpin B (9)	536	C ₂₈ H ₄₀ O ₁₀	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	7
Caesalpin MA (10)	390	C ₂₃ H ₃₄ O ₅	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	8
Caesalpin MB (11)	392	C ₂₃ H ₃₆ O ₅	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	8
Caesalpin MC (12)	350	C ₂₁ H ₃₄ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	8
Caeminaxin A (13)	464	C ₂₅ H ₃₆ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), leaves, Qinzhou, Guangxi Zhuang Autonomous Region, China	MeOH/EtOAc	9
Caeminaxin B (14)	466	C ₂₄ H ₃₄ O ₉	<i>Caesalpinia minax</i> Hance, (Fabaceae), leaves, Qinzhou, Guangxi Zhuang Autonomous Region, China	MeOH/EtOAc	9
Pterolobirin J (15)	318	C ₂₀ H ₃₀ O ₃	<i>Pterolobium macropterum</i> Kurz., (Fabaceae), roots, Silapet, Pua, Nan, Thailand	Acetone	10
Welwitschianic acid (16)	364	C ₂₁ H ₃₂ O ₅	<i>Caesalpinia welwitschiana</i> Oliv., (Fabaceae), liana, Mararaba village, East Cameroon	MeOH	11
Caesalpulcherrin I (17)	496	C ₂₉ H ₃₆ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtOAc	12
16-O-Methyl-cass-13(15)ene-16,18-dioic acid (18)	348	C ₂₁ H ₃₂ O ₄	<i>Parkia bicolor</i> A. Chev. (Fabaceae), stem roots, Adiopodoumé (Abidjan) in the south-central Cote d'Ivoire	80% MeOH/25% Diaion HP-20 column	13

Erythrofordin D (19)	348	C ₂₁ H ₃₂ O ₄	<i>Erythrophleum suaveolens</i> (Guill. et Perr.) Brenan, (Fabaceae), root barks, Cameroon	MeOH/EtOAc/Me OH (7:3)	14
Erythrofordin E (20)	346	C ₂₁ H ₃₀ O ₄	<i>Erythrophleum suaveolens</i> (Guill. et Perr.) Brenan, (Fabaceae), root barks, Cameroon	MeOH/EtOAc/Me OH (7:3)	14
6 α -Hydroxy-cassamic acid (21)	378	C ₂₁ H ₃₀ O ₆	<i>Erythrophleum suaveolens</i> (Guill. et Perr.) Brenan, (Fabaceae), root barks, Toumodi (Cote d ^ 'Ivoire)	MeOH/EtOAc	2
Erythrocasanoid A (22)	336	C ₂₀ H ₃₂ O ₄	<i>Erythrophleum fordii</i> Oliver, (Leguminosae), roots, Guangxi, China	95% EtOH/EtOAc	15
Erythrocasanoid B (23)	322	C ₂₀ H ₃₄ O ₃	<i>Erythrophleum fordii</i> Oliver, (Leguminosae), roots, Guangxi, China	95% EtOH/EtOAc	15
Erythrocasanoid D (24)	350	C ₂₀ H ₃₀ O ₅	<i>Erythrophleum fordii</i> Oliver, (Leguminosae), roots, Guangxi, China	95% EtOH/EtOAc	15
Erythrocasanoid E (25)	320	C ₂₀ H ₃₂ O ₃	<i>Erythrophleum fordii</i> Oliver, (Leguminosae), roots, Guangxi, China	95% EtOH/EtOAc	15
3-O- β -D-Galactopyranosyl-erythrosuamic acid methyl ester (26)	570	C ₂₈ H ₄₂ O ₁₂	<i>Erythrophleum suaveolens</i> (Guill. et Perr.) Brenan, (Fabaceae), seeds and root bark, Toumodi (Côte d'Ivoire)	MeOH/EtOAc	16
Caesmimo A1 (27)	288	C ₂₀ H ₃₂ O	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo A2 (28)	316	C ₂₁ H ₃₂ O ₂	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo A3 (29)	376	C ₂₂ H ₃₂ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo A4 (30)	378	C ₂₂ H ₃₄ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo A5 (31)	376	C ₂₂ H ₃₂ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo A6 (32)	374	C ₂₂ H ₃₀ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo A11 (33)	334	C ₂₀ H ₃₀ O ₄	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Capulchemin H (34)	486	C ₂₈ H ₃₈ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
Capulchemin I (35)	440	C ₂₇ H ₃₆ O ₅	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
Capulchemin J (36)	408	C ₂₇ H ₃₆ O ₃	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
4 β ,15-Dicarboxymethyl-12-oxocassa-13(14)-diene (37)	376	C ₂₂ H ₃₂ O ₅	<i>Pterolobium macropterum</i> Kurz, (Fabaceae), Funing, Yunnan, China	95% EtOH	19
Pulchin A (38)	424	C ₂₇ H ₃₆ O ₄	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yunnan, China	MeOH/EtOAc	20

Table S2. Biological activities of the most active cassane diterpenoids.

Compound	Activity	Ref.
Caesalpin MC (12)	Anti-inflammatory activity by prohibiting LPS-produced NO formation (inhibition rate 67.3%) in RAW 264.7 cells compared to dexamethasone (inhibition rate 51.2%), It reduced iNOS activity.	7
Caeminaxin A (13)	Anti-inflammation capacity by inhibiting MAPK phosphorylation and NF- κ B signaling pathway activation	9
19-Norneocassa-1,12(13),15-triene-3,14-dione (40)	Fungicidal potential against strawberry pathogens: <i>Colletotrichum fragariae</i> , <i>Colletotrichum acutatum</i> , and <i>Colletotrichum gloeosporioides</i>	21
14-Hydroxyneocassa- 1,12(17),15-triene-3-one (41)	Highest phytotoxic activity against creeping bentgrass	21
Norcaesalpinin O (59)	Phosphodiesterase-4B inhibition	22
Caesmimo B3 (62)	Anti-renal fibrosis activity by inhibiting fibronectin and collagen I expression induced by TGF- β 1 (transforming growth factor- β 1) in NRK-52E cells.	23
Voucapane WA (67)	Anti-inflammatory activity by inhibiting the excessive NO production (inhibition rate 66.1%) compared to dexamethasone (inhibition rate 51.2%) through suppressing iNOS enzymatic activation	24
17-Acetylcaesalmin Z (77)	Lipid lowering effect: significantly $\downarrow$ lipid accumulation in P/O-treated AML12 hepatocytes $\downarrow$ triglycerides and total cholesterol contents in P/O-treated AML12 hepatocytes	7
Capulchemin A (90)	Significantly controlled kiwifruit canker <i>in vivo</i> by destroying the cell membrane, leading to cell death. Potent antibacterial activity versus <i>Pseudomonas syringae</i> pv. <i>actinidae</i> and <i>Bacillus cereus</i> (MICs 3.13 μ M)	18
6 β -Acetoxysteroloterin A (113)	Significantly suppressed the production of NO (IC ₅₀ 7.18 μ M) in LPS-boosted BV-2 microglial cells	19
Caesalpinaxin (114)	Wound healing activity by stimulating migration and tuber generation in HUVECs through raising the VEGF level.	25
Cass-13(15)-en-16,12-olide (134)	PTP1B inhibitory potential (IC ₅₀ 217.45 μ M), compared to suramin sodium (IC ₅₀ 195.08 μ M)	26
14 β -hydroxycassa-11(12),13(15)-dien-12,16-olide (137)	Powerful α -glucosidase inhibitory capacity (IC ₅₀ 66 μ M); acarbose (IC ₅₀ 178 μ M)	27
Phanginin JA (146)	Marked antiproliferative potential (IC ₅₀ 16.79 μ M) versus A549 cells and induced apoptosis by suppressing G0/G1 phase cell cycle	4
Caesalpulcherrin K (179)	Inhibition against LPS-induced NO production in BV-2 microglial cells (IC ₅₀ 6.34 μ M), compared to quercetin (IC ₅₀ 2.4 μ M).	28
Caesalpulcherrin L (180)	Inhibition against LPS-induced NO production in BV-2 microglial cells (IC ₅₀ 6.04 μ M), compared to quercetin (IC ₅₀ 2.4 μ M)	28
Caesalpulcherrin M (181)	Inhibition against LPS-induced NO production in BV-2 microglial cells (IC ₅₀ 6.48 μ M), compared to quercetin (IC ₅₀ 2.4 μ M)	28
6'-Acetoxysterolobirin B (204)	Potent α -glucosidase inhibition capacity; acarbose (IC ₅₀ 178 μ M)	27
Biscaesalmin A (206)	Anti-inflammatory activity by suppressing LPS-caused NO formation in THP-1 macrophages.	29
Biscaesalmin B (207)	Anti-inflammatory activity by suppressing LPS-caused NO formation in THP-1 macrophages. It prohibited macrophage migration towards adipocytes and suppressed NLRP3 inflammasome-mediated IL-1 β production.	29
Sappamide BC (210)	Anti-inflammatory activity by inhibiting the excessive NO production	30

	through the reduction of iNOS enzyme activity and iNOS protein expression downregulation.	
Caesanamides A (225) and B (226)	Cytotoxic effectiveness versus MCF-7 cell line (IC ₅₀ s 27.23 and 29.67 μ M, respectively), compared to cisplatin (IC ₅₀ 16.95 μ M)	31
Bokkosin (237)	Powerful anti- <i>Trypanosomal</i> activity against <i>T. brucei brucei</i>	32

Table S3: List of new neocassane and norcassane diterpenoids reported from 2019 to 2025.

Compound Name/Chemical Class	M. Wt.	Mol. Formula	Plant, Family, Part used, and Location	Extract/Fraction	Ref.
Neocassane diterpenoids					
Neocassa-1,12(13),15-triene-3,14-dione (39)	298	C ₂₀ H ₂₆ O ₂	<i>Eragrostis plana</i> Nees, (Poaceae), leaves and roots, city of Passo Fundo, Rio Grande do Sul state, Brazil	MeOH:CH ₂ Cl ₂ /Hexane	21
19-Norneocassa-1,12(13),15-triene-3,14-dione (40)	284	C ₁₉ H ₂₄ O ₂	<i>Eragrostis plana</i> Nees, (Poaceae), leaves and roots, city of Passo Fundo, Rio Grande do Sul state, Brazil	MeOH:CH ₂ Cl ₂ /Hexane	21
14-Hydroxyneocassa-1,12(17),15-triene-3-one (41)	300	C ₂₀ H ₂₈ O ₂	<i>Eragrostis plana</i> Nees, (Poaceae), leaves and roots, city of Passo Fundo, Rio Grande do Sul state, Brazil	MeOH:CH ₂ Cl ₂ /Hexane	21
Norcassane diterpenoids					
Erythro-norcassanoid A (42)	306	C ₁₉ H ₃₀ O ₃	<i>Erythrophleum fordii</i> Oliver, (Leguminosae), roots, Guangxi, China	95% EtOH/EtOAc	15
Erythro-norcassanoid B (43)	336	C ₁₉ H ₂₈ O ₅	<i>Erythrophleum fordii</i> Oliver, (Leguminosae), roots, Guangxi, China	95% EtOH/EtOAc	15
Norcaesalpin MD (44)	318	C ₂₀ H ₃₀ O ₃	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	8
Norcaesalpin ME (45)	292	C ₁₈ H ₂₈ O ₃	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	8
Norcaesalpin MG (46)	318	C ₁₉ H ₂₆ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Malipo, Yunnan, China	75% EtOH/CHCl ₃	33
Norcaesalpin MF (47)	344	C ₂₁ H ₂₈ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	8
Capulchemin K (48)	428	C ₂₅ H ₃₂ O ₆	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
Distemonanthin (49)	336	C ₁₉ H ₂₈ O ₅	<i>Distemonanthus benthamianus</i> Baill. (Fabaceae), stem barks, West Region of Cameroon	MeOH/EtOAc	34
Caesmimo A7 (50)	318	C ₂₀ H ₃₀ O ₃	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo A8 (51)	332	C ₂₁ H ₃₂ O ₃	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo A10 (52)	304	C ₁₉ H ₂₈ O ₃	<i>Caesalpinia mimosoides</i> Lam.,	75% EtOH/CHCl ₃	17

			(Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China		
Caesalpanin D (53)	302	C ₁₉ H ₂₆ O ₃	<i>Caesalpinia sappan</i> L., (Fabaceae), Seeds, Baise, Guangxi, China	95% EtOH/EtOAc	35
Caesalpanin E (54)	344	C ₂₀ H ₂₄ O ₅	<i>Caesalpinia sappan</i> L., (Fabaceae), Seeds, Baise, Guangxi, China	95% EtOH/EtOAc	35
Caesalpinin JA (55)	300	C ₁₉ H ₂₄ O ₃	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	95% EtOH/CHCl ₃	31
Caesalminaxin T (56)	374	C ₂₁ H ₂₆ O ₆	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Qingping herbal medicine market, Guangdong, China	MeOH/CHCl ₃	36
6 α -Hydroxynorcaesalpinin A (57)	434	C ₂₃ H ₃₀ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	7
Norcaesalpinin ME (58)	434	C ₂₃ H ₃₀ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	7
Norcaesalpinin O (59)	360	C ₂₁ H ₂₈ O ₅	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	75% EtOH/CHCl ₃	22
Norcaesalpinin P (60)	418	C ₂₃ H ₃₀ O ₇	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	75% EtOH/CHCl ₃	22
Norcaesalpinin Q (61)	392	C ₂₁ H ₂₈ O ₇	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	75% EtOH/CHCl ₃	37
Caesmimo B3 (62)	388	C ₂₂ H ₂₈ O ₆	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23
Caesmimo B4 (63)	388	C ₂₂ H ₂₈ O ₆	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23
Norvoucapane FA (64)	344	C ₂₁ H ₂₈ O ₄	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	75% EtOH/petroleum ether	24
Norvoucapane FC (65)	302	C ₁₉ H ₂₆ O ₃	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	75% EtOH/petroleum ether	24
Pterolobirin E (66)	286	C ₁₉ H ₂₆ O ₂	<i>Pterolobium macropterum</i> Kurz., (Fabaceae), roots, Silapet, Pua, Nan, Thailand	Acetone	10

Table S4: List of cassane furanoditerpenoids reported from 2019 to 2025.

Compound Name	M. Wt.	Mol. Formula	Plant, Family, Part used, and Location	Extract/Fraction	Ref.
Voucapane WA (67)	390	C ₂₃ H ₃₄ O ₅	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	75% EtOH/petroleum ether	24
Voucapane WB (68)	374	C ₂₃ H ₃₄ O ₄	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	75% EtOH/petroleum ether	24
Voucapane WD (69)	356	C ₂₂ H ₂₈ O ₄	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	75% EtOH/petroleum ether	24
Voucapane WE (70)	374	C ₂₃ H ₃₄ O ₄	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	EtOH/Petroleum ether	1
Caesalminaxin P (71)	464	C ₂₅ H ₃₆ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Qingping herbal medicine market, Guangdong, China	MeOH/CHCl ₃	36
Caesalminaxin Q (72)	464	C ₂₅ H ₃₆ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Qingping herbal medicine market, Guangdong, China	MeOH/CHCl ₃	36
Caesalminaxin R (73)	464	C ₂₄ H ₃₂ O ₉	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Qingping herbal medicine market, Guangdong, China	MeOH/CHCl ₃	36
Caesalminaxin S (74)	480	C ₂₅ H ₃₆ O ₉	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Qingping herbal medicine market, Guangdong, China	MeOH/CHCl ₃	36
6-Deacetylcaesalmin Z (75)	408	C ₂₂ H ₃₂ O ₇	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	85% EtOH/EtOAc	38
14- <i>epi</i> -Caesalmin Z (76)	466	C ₂₄ H ₃₄ O ₉	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	85% EtOH/EtOAc	38
17-Acetylcaesalmin Z (77)	508	C ₂₆ H ₃₆ O ₁₀	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	7
Sucupiranin MA (78)	284	C ₂₀ H ₂₈ O	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	EtOH/Petroleum ether	1
Pterolobirin C (78) = Sucupiranin MA	284	C ₂₀ H ₂₈ O	<i>Pterolobium macropterum</i> Kurz., (Fabaceae), roots, Silapet, Pua, Nan, Thailand	Acetone	10
Sucupiranin MB (79)	342	C ₂₂ H ₃₀ O ₃	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	75% EtOH/petroleum ether	24
Sucupiranin MC (80)	300	C ₂₀ H ₂₈ O ₂	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	75% EtOH/petroleum ether	24
14- <i>epi</i> -Caesalpinin E1 (81)	392	C ₂₂ H ₃₂ O ₆	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous	85% EtOH/EtOAc	38

Region, China					
Caesalpinin JB (82)	388	C ₂₂ H ₂₈ O ₆	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	95% EtOH/CHCl ₃	31
Caesalpinin JC (83)	330	C ₂₀ H ₂₆ O ₄	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	95% EtOH/CHCl ₃	31
Caesalpinin JD (84)	388	C ₂₂ H ₂₈ O ₆	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	95% EtOH/CHCl ₃	31
Caesalpinin MQ (85)	474	C ₂₆ H ₃₄ O ₈	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	75% EtOH/CHCl ₃	22
6 α -Hydroxycasalpinin P (86)	432	C ₂₄ H ₃₂ O ₇	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	85% EtOH/EtOAc	38
Caesalpinin MR (87)	392	C ₂₂ H ₃₂ O ₆	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	75% EtOH/CHCl ₃	37
Caesalpanin F (88)	358	C ₂₁ H ₂₆ O ₅	<i>Caesalpinia sappan</i> L., (Fabaceae), Seeds, Baise, Guangxi, China	95% EtOH/EtOAc	35
Caesappine B (89)	374	C ₂₂ H ₃₀ O ₅	<i>Caesalpinia sappan</i> L., (Fabaceae), Seeds, Nanning, Guangxi, China	MeOH/CHCl ₃	39
Capulchemin A (90)	534	C ₃₁ H ₃₄ O ₈	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
Capulchemin B (91)	508	C ₂₉ H ₃₂ O ₈	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
Capulchemin C (92)	476	C ₂₉ H ₃₂ O ₆	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
Capulchemin D (93)	418	C ₂₇ H ₃₀ O ₄	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
Capulchemin E (94)	448	C ₂₇ H ₂₈ O ₆	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
Capulchemin F (95)	444	C ₂₉ H ₃₂ O ₄	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtOAc	18
Caesamin A (96)	456	C ₂₇ H ₃₆ O ₆	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Anguo market of material medica, Hebei, China	Acetone	5
Caesamin B (97)	462	C ₂₄ H ₃₀ O ₉	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Anguo market of material medica, Hebei, China	Acetone	5
Caesamin C (98)	462	C ₂₄ H ₃₀ O ₉	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Anguo market of material medica, Hebei, China	Acetone	5
Pterolobirin D (99)	342	C ₂₂ H ₃₀ O ₃	<i>Pterolobium macropterum</i> Kurz., (Fabaceae), roots, Silapet, Pua, Nan, Thailand	Acetone	10
Pterolobirin F (100)	314	C ₂₀ H ₂₆ O ₃	<i>Pterolobium macropterum</i> Kurz., (Fabaceae), roots, Silapet, Pua, Nan, Thailand	Acetone	10
Caesmimo B1 (101)	388	C ₂₃ H ₃₂ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23
Caesmimo B2 (102)	386	C ₂₃ H ₃₀ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23

			(Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China		
Caesalbonducin O (103)	448	C ₂₄ H ₃₂ O ₈	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOAc	6
Caesalbonducin P (104)	404	C ₂₂ H ₂₈ O ₇	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOAc	6
Cassabonducin C (105)	314	C ₂₀ H ₂₆ O ₃	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
Cassabonducin D (106)	418	C ₂₄ H ₃₄ O ₆	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
Cassabonducin E (107)	418	C ₂₄ H ₃₄ O ₆	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
Cassabonducin F (108)	432	C ₂₄ H ₃₂ O ₇	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
Cassabonducin G (109)	448	C ₂₄ H ₃₂ O ₈	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
Cassabonducin H (110)	422	C ₂₃ H ₃₄ O ₇	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
Cassabonducin I (111)	436	C ₂₃ H ₃₂ O ₈	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
Cassabonducin J (112)	494	C ₂₅ H ₃₄ O ₁₀	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
6β-Acetoxypteroloterin A (113)	428	C ₂₄ H ₂₈ O ₇	<i>Pterolobium macropterum</i> Kurz, (Fabaceae), Funing, Yunnan, China	95% EtOH	19
Caesalpinaxin (114)	458	C ₂₅ H ₃₀ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping County, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	25

Table S5: List of cassane dihydrofuran diterpenoids reported from 2019 to 2025.

Compound Name	M. Wt.	Mol. Formula	Plant, Family, Part used, and Location	Extract/Fraction	Ref.
Caesalpulcherrin A (115)	500	C ₂₉ H ₄₀ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtOAc	12
Caesalpulcherrin B (116)	526	C ₃₁ H ₄₂ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtOAc	12
Caesalpulcherrin C (117)	526	C ₃₁ H ₄₂ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtOAc	12
Caesalpulcherrin D (118)	526	C ₃₁ H ₄₂ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtOAc	12
Caesalpulcherrin E (119)	678	C ₃₇ H ₄₂ O ₁₂	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtOAc	12
Caesalpulcherrin F (120)	468	C ₂₈ H ₃₆ O ₆	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtOAc	12
Pulchin B (121)	634	C ₃₆ H ₄₂ O ₁₀	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yunnan, China	MeOH/EtOAc	20
Caesalminaxin HA (122)	404	C ₂₄ H ₃₆ O ₅	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	EtOH/Petroleum ether	1
Caesalminaxin HC (123)	332	C ₂₁ H ₃₂ O ₃	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	41
Caesalminaxin HD (124)	374	C ₂₃ H ₃₄ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	41
Caesalminaxin O (125)	524	C ₂₇ H ₄₀ O ₁₀	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Qingping herbal medicine market, Guangdong, China	MeOH/CHCl ₃	36
Pterolobirin G (126)	300	C ₂₀ H ₂₈ O ₂	<i>Pterolobium macropterum</i> Kurz., (Fabaceae), roots, Silapet, Pua, Nan, Thailand	Acetone	10
Caesall FE (127)	372	C ₂₃ H ₃₂ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	41
Caesall O (128)	374	C ₂₂ H ₃₀ O ₅	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	75% EtOH/CHCl ₃	22
Caesall P (129)	374	C ₂₂ H ₃₀ O ₅	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	75% EtOH/CHCl ₃	22
Cassabonducin B (130)	474	C ₂₆ H ₃₄ O ₈	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
ε-Caesalpin-VII (131)	416	C ₂₄ H ₃₂ O ₆	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40

Table S6: List of cassane diterpenoids with fused butenolide moiety reported from 2019 to 2025.

Compound Name	M. Wt.	Mol. Formula	Plant, Family, Part used, and Location	Extract/Fraction	Ref.
Erythrocassanoid C (132)	348	C ₂₀ H ₂₈ O ₅	<i>Erythrophleum fordii</i> Oliver, (Leguminosae), roots, Guangxi, China	95% EtOH/EtOAc	15
Neocawsalpin WM (133)	350	C ₂₀ H ₃₀ O ₅	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Malipo, Yunnan, China	75% EtOH/CHCl ₃	33
Sucutinirane SA (134) = Cass-13(15)-en-16,12-olide (134)	302	C ₂₀ H ₃₀ O ₂	<i>Caesalpinia cucullata</i> Roxb., (Fabaceae), seed kernels, Yunnan, China	75% EtOH/petroleum ether	24
	302	C ₂₀ H ₃₀ O ₂	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seeds, Chongzuo, Guangxi Zhuang Autonomous Region, China	95% EtOH	26
(4 <i>S</i>)-6β,12α,19-Trihydroxy-cass-13(15)-en-16,12-olide (135)	350	C ₂₀ H ₃₀ O ₅	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seeds, Chongzuo, Guangxi Zhuang Autonomous Region, China	95% EtOH	26
12α-Hydroxy-cass-13(15)-en-16,12-olide (136)	318	C ₂₀ H ₃₀ O ₃	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seeds, Chongzuo, Guangxi Zhuang Autonomous Region, China	95% EtOH	26
14β-Hydroxycassa-11(12),13(15)-dien-12,16-olide (137)	312	C ₂₀ H ₂₈ O ₂	<i>Pterolobium macropterum</i> Kurz, (Fabaceae), fruits, Song Khwae District, Nan, Thailand	MeOH	27
Caesmimo A12 (138)	376	C ₂₂ H ₃₂ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo A13 (139)	376	C ₂₂ H ₃₂ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17
Caesmimo C1 (140)	360	C ₂₁ H ₂₈ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23
Caesmimo C2 (141)	360	C ₂₁ H ₂₈ O ₅	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23
Caesmimo C6 (142)	392	C ₂₂ H ₃₂ O ₆	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23
Caesmimo C7 (143)	378	C ₂₁ H ₃₀ O ₆	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23
Caesmimo C9 (144)	434	C ₂₄ H ₃₄ O ₇	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23
Caesmimo C10 (145)	406	C ₂₃ H ₃₄ O ₆	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	23
Phanginin JA (146)	448	C ₂₄ H ₃₂ O ₈	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, Qinzhou, Guangxi, China	95% EtOH/CHCl ₃	4
Phanginin JB (147)	406	C ₂₂ H ₃₀ O ₇	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, Qinzhou, Guangxi, China	95% EtOH/CHCl ₃	4

Phanginin JC (148)	402	C ₂₂ H ₂₆ O ₇	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, Qinzhou, Guangxi, China	95% EtOH/CHCl ₃	4
Phanginin JD (149)	406	C ₂₂ H ₃₀ O ₇	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, Qinzhou, Guangxi, China	95% EtOH/CHCl ₃	4
Phanginin JE (150)	406	C ₂₂ H ₃₀ O ₇	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, Qinzhou, Guangxi, China	95% EtOH/CHCl ₃	4
Caesalpinolide H (151)	464	C ₂₄ H ₃₂ O ₉	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	3
Caesalpinolide I (152)	506	C ₂₆ H ₃₄ O ₁₀	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	85% EtOH/EtOAc	38
Caesalpinolide J (153)	448	C ₂₄ H ₃₂ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	3
Caesalpinolide K (154)	552	C ₂₇ H ₃₆ O ₁₂	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	85% EtOH/EtOAc	38
Caesalpinolide L (155)	450	C ₂₃ H ₃₀ O ₉	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	85% EtOH/EtOAc	38
Caesalpinolide M (156)	508	C ₂₆ H ₃₆ O ₁₀	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	85% EtOH/EtOAc	38
Caesalpinolide N (157)	494	C ₂₆ H ₃₈ O ₉	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	85% EtOH/EtOAc	38
12-O-Ethyl neocaesalpin B (158)	478	C ₂₆ H ₃₈ O ₈	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	3
14- <i>epi</i> -Neocaesalpin L (159)	524	C ₂₆ H ₃₆ O ₁₁	<i>Caesalpinia bonduc</i> (L.) Roxb., (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	85% EtOH/EtOAc	38
Neocaesalpin WA (160)	316	C ₂₀ H ₂₈ O ₃	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WB (161)	358	C ₂₂ H ₃₀ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WC (162)	332	C ₂₀ H ₂₈ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WD (163)	348	C ₂₁ H ₃₂ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WE (164)	364	C ₂₁ H ₃₂ O ₅	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WF (165)	390	C ₂₃ H ₃₄ O ₅	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WG (166)	332	C ₂₁ H ₃₂ O ₃	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WH (167)	318	C ₂₀ H ₃₀ O ₃	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WI (168)	334	C ₂₀ H ₃₀ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WJ (169)	360	C ₂₂ H ₃₂ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Neocaesalpin WK (170)	360	C ₂₂ H ₃₂ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30

Neocaesalpin WL (171)	360	C ₂₂ H ₃₂ O ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
12-Demethylcaesalpin G (172)	406	C ₂₂ H ₃₀ O ₇	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	3
12-Demethylcaesalpin H (173)	464	C ₂₄ H ₃₂ O ₉	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Zhaoping, Guangxi Zhuang Autonomous Region, China	95% EtOH/CHCl ₃	3
Caesalpinin JE (174)	436	C ₂₃ H ₃₂ O ₈	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	95% EtOH/CHCl ₃	31
Cassabonducin A (175)	488	C ₂₆ H ₃₂ O ₉	<i>Caesalpinia bonduc</i> (Linn.) Roxb., (Fabaceae), seeds, Anguo market of material medica, Hebei, China	95% EtOH	40
Caesalpulcherrin G (176)	662	C ₃₆ H ₃₈ O ₁₂	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtO Ac	12
Caesalpulcherrin H (177)	484	C ₂₈ H ₃₆ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtO Ac	12
Caesalpulcherrin J (178)	486	C ₂₈ H ₃₈ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtO Ac	12
Caesalpulcherrin K (179)	494	C ₂₉ H ₃₄ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtO AC	28
Caesalpulcherrin L (180)	496	C ₂₉ H ₃₆ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtO AC	28
Caesalpulcherrin M (181)	408	C ₂₂ H ₃₂ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat town, Binh Duong Province, Viet Nam	MeOH/EtO AC	28
Pulcherritam E (182)	422	C ₂₃ H ₃₄ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat, Binh Duong, Viet Nam	MeOH/EtO Ac	42
Pulcherritam F (183)	454	C ₂₇ H ₃₄ O ₆	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat, Binh Duong, Viet Nam	MeOH/EtO Ac	42
Pulcherritam G (184)	524	C ₂₉ H ₃₂ O ₉	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat, Binh Duong, Viet Nam	MeOH/EtO Ac	42
Pulcherritam H (185)	586	C ₃₄ H ₃₄ O ₉	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat, Binh Duong, Viet Nam	MeOH/EtO Ac	42
Caesalatic acid A (186)	448	C ₂₅ H ₃₆ O ₇	<i>Caesalpinia latisiliqua</i> (Cav.) Hattink, leaves, Ngoc Thanh, Phuc Yen, Vinh Phuc, Vietnam	MeOH/CH ₂ Cl ₂	43
Caesalatic acid B (187)	432	C ₂₅ H ₃₆ O ₆	<i>Caesalpinia latisiliqua</i> (Cav.) Hattink, leaves, Ngoc Thanh, Phuc Yen, Vinh Phuc, Vietnam	MeOH/CH ₂ Cl ₂	43
Caesappine A (188)	538	C ₂₇ H ₃₈ O ₁₁	<i>Caesalpinia sappan</i> L., (Fabaceae), Seeds, Nanning, Guangxi, China	MeOH/CHCl ₃	39
Capulchemin G (189)	542	C ₂₉ H ₃₄ O ₁₀	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), stems, Yun, China	MeOH/EtO Ac	18
Caesalbonducin K (190)	552	C ₂₈ H ₄₀ O ₁₁	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae),	95%	6

			pericarps, Zhanjiang, Guangdong, China	EtOH/EtOA c	
Caesalbonducin L (191)	552	C ₂₈ H ₄₀ O ₁₁	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOA c	6
Caesalbonducin M (192)	494	C ₂₆ H ₃₈ O ₉	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOA c	6
Caeslpulrin A (193)	470	C ₂₇ H ₃₄ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), fruits, Xishuangbanna, Yunnan, China	EtOH/EtOA c	44
Caeslpulrin B (194)	512	C ₂₉ H ₃₆ O ₈	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), fruits, Xishuangbanna, Yunnan, China	EtOH/EtOA c	44
Caeslpulrin C (195)	454	C ₂₇ H ₃₄ O ₆	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), fruits, Xishuangbanna, Yunnan, China	EtOH/EtOA c	44
Caeslpulrin D (196)	496	C ₂₉ H ₃₆ O ₇	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), fruits, Xishuangbanna, Yunnan, China	EtOH/EtOA c	44
Caeslpulrin E (197)	452	C ₂₇ H ₃₂ O ₆	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), fruits, Xishuangbanna, Yunnan, China	EtOH/EtOA c	44
Caeslpulrin F (198)	552	C ₃₁ H ₃₆ O ₉	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), fruits, Xishuangbanna, Yunnan, China	EtOH/EtOA c	44
Caeslpulrin G (199)	632	C ₃₆ H ₄₀ O ₁₀	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), fruits, Xishuangbanna, Yunnan, China	EtOH/EtOA c	44
Pterolobirin H (200)	298	C ₂₀ H ₂₆ O ₂	<i>Pterolobium macropterum</i> Kurz., (Fabaceae), roots, Silapet, Pua, Nan, Thailand	Acetone	10
Pterolobirin I (201)	318	C ₂₀ H ₃₀ O ₃	<i>Pterolobium macropterum</i> Kurz., (Fabaceae), roots, Silapet, Pua, Nan, Thailand	Acetone	10

Table S7: Occurrence of cassane diterpenoid dimers and penta-spiro cassane diterpenoids from 2019 to 2025.

Compound Name/Chemical Class	M. Wt.	Mol. Formula	Plant, Family, Part used, and Location	Extract/Fraction	Ref.
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Cassane diterpenoid dimers					
Pterolobirin A (202)	616	C ₄₀ H ₅₆ O ₅	<i>Pterolobium macropterum</i> Kurz, (Fabaceae), fruits, Silapet, Pua, Nan Province, Thailand	MeOH/EtOAc	45
Pterolobirin B (203)	674	C ₄₂ H ₅₈ O ₇	<i>Pterolobium macropterum</i> Kurz, (Fabaceae), fruits, Silapet, Pua, Nan Province, Thailand	MeOH/EtOAc	45
6'-Acetoxypterolobirin B (204)	732	C ₄₄ H ₆₀ O ₉	<i>Pterolobium macropterum</i> Kurz, (Fabaceae), fruits, Song Khwae District, Nan, Thailand	MeOH	27
Caesalpanin C (205)	704	C ₄₂ H ₅₆ O ₉	<i>Caesalpinia sappan</i> L., (Fabaceae), Seeds, Baise, Guangxi, China	95% EtOH	46
Biscaesalmin A (206)	878	C ₄₈ H ₆₂ O ₁₅	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, China	95% EtOH/CHCl ₃	29
Biscaesalmin B (207)	806	C ₄₆ H ₆₂ O ₁₂	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, China	95% EtOH/CHCl ₃	29
Penta-spiro cassane diterpenoids					
Caesalatic acid C (208)	448	C ₂₅ H ₃₆ O ₇	<i>Caesalpinia latisiliqua</i> (Cav.) Hattink, (Fabaceae), leaves, Ngoc Thanh, Phuc Yen, Vinh Phuc, Vietnam	MeOH/CH ₂ Cl ₂	43
Caesmimo A9 (209)	378	C ₂₁ H ₃₀ O ₆	<i>Caesalpinia mimosoides</i> Lam., (Fabaceae), seeds, mountain near Fapa Hot Spring in Dehong, Yunnan, China	75% EtOH/CHCl ₃	17

Table S8: Occurrence of cassane diterpenoid alkaloids from 2019 to 2025.

Compound Name	M. Wt.	Mol. Formula	Plant, Family, Part used, and Location	Extract/Fraction	Ref.
Sappamide BC (210)	315	C ₂₀ H ₂₉ NO ₂	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Sappamide BD (211)	373	C ₂₂ H ₃₁ NO ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Sappamide BE (212)	373	C ₂₂ H ₃₁ NO ₄	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Sappamide AD (213)	361	C ₂₂ H ₃₅ NO ₃	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Sappamide CI (214)	333	C ₂₀ H ₃₁ NO ₃	<i>Caesalpinia sinensis</i> (Hemsl.) Vidal, (Fabaceae), seed kernels, Yunnan, China	75% EtOH/CHCl ₃	30
Caesamin D (215)	523	C ₂₆ H ₃₇ NO ₁₀	<i>Caesalpinia minax</i> Hance, (Fabaceae), seeds, Anguo market of material medica, Hebei, China	Acetone	5
Caesalminine C (216)	631	C ₃₂ H ₄₁ NO ₁₂	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOAc	6
Caesalminine D (217)	573	C ₃₀ H ₃₉ NO ₁₀	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOAc	6
Caesalminine D (218)	531	C ₂₈ H ₃₇ NO ₉	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOAc	6
Caesalminine F (219)	487	C ₂₆ H ₃₃ NO ₈	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOAc	6
Caesalminine G (220)	489	C ₂₆ H ₃₅ NO ₈	<i>Caesalpinia bonduc</i> (L.) Roxb, (Fabaceae), pericarps, Zhanjiang, Guangdong, China	95% EtOH/EtOAc	6
Pulcherritam A (221)	483	C ₂₈ H ₃₇ NO ₆	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat, Binh Duong, Viet Nam	MeOH/EtOAc	42
Pulcherritam B (222)	477	C ₂₉ H ₃₅ NO ₅	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat, Binh Duong, Viet Nam	MeOH/EtOAc	42
Pulcherritam C (223)	451	C ₂₇ H ₃₃ NO ₅	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat, Binh Duong, Viet Nam	MeOH/EtOAc	42
Pulcherritam D (224)	389	C ₂₂ H ₃₁ NO ₅	<i>Caesalpinia pulcherrima</i> L., (Fabaceae), aerial parts, Ben Cat, Binh Duong, Viet Nam	MeOH/EtOAc	42
Caesanamide A (225)	399	C ₂₃ H ₂₉ NO ₅	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, An Guo	95% EtOH/CHCl ₃	31

			Medicinal Material Corporation, Hebei, China		
Caesanamide B (226)	441	C ₂₅ H ₃₁ NO ₆	<i>Caesalpinia sappan</i> L., (Fabaceae), seeds, An Guo Medicinal Material Corporation, Hebei, China	95% EtOH/CHCl ₃	31
Caesalpanin A (227)	701	C ₄₂ H ₅₅ NO ₈	<i>Caesalpinia sappan</i> L., (Fabaceae), Seeds, Baise, Guangxi, China	95% EtOH	46
Caesalpanin B (228)	689	C ₄₂ H ₅₉ NO ₇	<i>Caesalpinia sappan</i> L., (Fabaceae), Seeds, Baise, Guangxi, China	95% EtOH	46

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