

Presence of Compounds in Manacá (*Brunfelsia grandiflora*)

Compound	Chemical Type	Plant Part	Plant Origin	Quantity	Ref #
Acetone	Alkanone to C4	Aerial Parts	Switzerland	00.40%	K28911
Aesculetin	Coumarin	Root	Brazil	Not stated	W02597
Anisole, 4-methyl-	Benzenoid	Aerial Parts	Switzerland	00.03%	K28911
Benzaldehyde	Benzenoid	Aerial Parts	Switzerland	00.05%	K28911
Benzyl benzoate	Benzenoid	Aerial Parts	Switzerland	Traces	K28911
Benzyl salicylate	Benzenoid	Aerial Parts	Switzerland	Traces	K28911
Bisabolene, beta-	Sesquiterpene	Aerial Parts	Switzerland	00.04%	K28911
Brunfelsene		Plant	Not stated	Not stated	ZZ1095
Brunfelsamidine	Alkaloid	Rootbark	Peru	00.08889%	H00026
But-3-en-1-ol, 3-methyl-	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
But-3-en-2-one	Alkanone to C4	Aerial Parts	Switzerland	00.03%	K28911
But-3-en-2-one, 3-methyl-	Alkanone to C4	Aerial Parts	Switzerland	00.03%	K28911
Butan-1-al	Alkanal to C4	Aerial Parts	Switzerland	00.03%	K28911
Butan-1-al, 2-methyl-	Alkanal to C4	Aerial Parts	Switzerland	00.03%	K28911
Butan-1-al, 3-methyl-	Alkanal to C4	Aerial Parts	Switzerland	00.14%	K28911
Chromane, rel-4(a)-7-8-8-(a)-tetrahydro-1-1-3-6-tetramethyl-3-vinyl-iso-	Sesquiterpene	Aerial Parts	Switzerland	00.09%	K28911
Cyclocitral, beta-	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Cyclohex-1-3-diene, 2-6-6-trimethyl-	Alicyclic	Aerial Parts	Switzerland	00.03%	K28911
Cyclohex-2-en-1-one, 4-(2-butenylide)-3-5-5-trimethyl-	Alicyclic	Aerial Parts	Switzerland	00.06%	K28911
Cyclohexan-1-one, 2-2-6-trimethyl-	Alicyclic	Aerial Parts	Switzerland	00.03%	K28911
Damascenone, beta-	Sesquiterpene	Aerial Parts	Switzerland	00.06%	K28911
Decane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911

Compound	Chemical Type	Plant Part	Plant Origin	Quantity	Ref #
Elemol	Sesquiterpene	Aerial Parts	Switzerland	00.04%	K28911
Esculetin		Bark	Not stated	Not stated	ZZ1095
Eudesmol, beta-	Sesquiterpene	Aerial Parts	Switzerland	00.03%	K28911
Farnesol	Sesquiterpene	Aerial Parts	Switzerland	00.03%	K28911
Farnesol, 6-7-dihydro-	Sesquiterpene	Aerial Parts	Switzerland	Traces	K28911
Farnesyl-acetone	Sesquiterpene	Aerial Parts	Switzerland	00.10%	K28911
Furan, 2-ethyl-	Oxygen Heterocycle	Aerial Parts	Switzerland	00.05%	K28911
Furan, 2-pentyl-	Oxygen Heterocycle	Aerial Parts	Switzerland	00.03%	K28911
Furan, methyl-	Oxygen Heterocycle	Aerial Parts	Switzerland	00.03%	K28911
Furane, 5-(1-5-dimethyl-1-4-hexadienyl)-tetrahydro-2-methyl-2-vinyl-	Oxygen Heterocycle	Aerial Parts	Switzerland	Traces	K28911
Furosta-2-alpha-3-beta-22-26-tetraol,(5-alpha-25r)-26-o-beta-d-glucopyranoside	Sapogenin	Root	Brazil	00.00107%	H14972
Furosta-3-beta-22-26-triol, (5-alpha-25r)-26-o-beta-d-glucopyranosyl-22-o-methyl-hopamidine	Sapogenin	Root Leaf	Brazil South America	00.00064% 00.015%	H14972 K10192
Geraniol	Monoterpene	Aerial Parts	Switzerland	00.44%	K28911
Geranyl acetone	Sesquiterpene	Aerial Parts	Switzerland	00.18%	K28911
Heneicosane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911
Hept-5-en-2-ol, 6-methyl-	Alkenol C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Hept-5-en-2-one, 6-methyl-	Alkenone C5 or More	Aerial Parts	Switzerland	00.08%	K28911
Hept-cis-4-en-1-al	Alkenal C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Hept-trans-2-en-1-al	Alkenal C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Hepta-1-5-diene, trimethyl-	Alkene C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Hepta-2-4-dien-1-ol	Alkenol C5 or More	Aerial Parts	Switzerland	00.08%	K28911
Heptadecane, n-	Alkane C5 or More	Aerial Parts	Switzerland	traces	K28911
Heptan-1-al	Alkanal C5 or More	Aerial Parts	Switzerland	00.03%	K28911

Compound	Chemical Type	Plant Part	Plant Origin	Quantity	Ref #
Heptan-2-one	Alkanone C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Heptane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911
Hex-1-en-3-one	Alkenone C5 or More	Aerial Parts	Switzerland	Traces	K28911
Hex-cis-3-en-1-ol	Alkenol C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Hex-cis-3-en-1-ol salicylate	Alkenol C5 or More	Aerial Parts	Switzerland	00.26%	K28911
Hex-trans-2-en-1-al	Alkenal C5 or More	Aerial Parts	Switzerland	00.93%	K28911
Hex-trans-3-en-1-ol	Alkenol C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Hexadeca-7-10-13-trienoic acid methyl ester	Lipid	Aerial Parts	Switzerland	00.03%	K28911
Hexadecane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911
Hexan-1-al	Alkanal C5 or More	Aerial Parts	Switzerland	00.04%	K28911
Hexan-1-ol	Alkanol C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Hexan-1-ol, 2-ethyl-	Alkanol C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Hopeanine	Quinolizidine Alkaloid	Root Root Bark	Brazil Brazil Not stated	Not stated Not stated 4 ppm	T01443 T01415 ZZ1095
Ionol, alpha- trans-2-3-dehydro-	Sesquiterpene	Aerial Parts	Switzerland	00.04%	K28911
Ionone, alpha-	Sesquiterpene	Aerial Parts	Switzerland	00.09%	K28911
Ionone, beta-	Sesquiterpene	Aerial Parts	Switzerland	00.16%	K28911
Ionone, beta- trans-5-6-epoxy-	Sesquiterpene	Aerial Parts	Switzerland	00.06%	K28911
Kaempferol-3-o-(6-glc-o-feruloyl)-beta-d-gluco-pyranosyl(1-2)-o-[alpha-l-rhamnopyranosyl(1-6)]-beta-d-galactopyranoside	Flavonol	Aerial Parts	Switzerland	00.0101%	H25351
Lavandulal	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Limonene	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Linalool	Monoterpene	Aerial Parts	Switzerland	02.19%	K28911
Linalool oxide(furanoid)	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Linoleic acid methyl ester	Lipid	Aerial Parts	Switzerland	00.12%	K28911

Compound	Chemical Type	Plant Part	Plant Origin	Quantity	Ref #
Linolenic acid methyl ester	Lipid	Aerial Parts	Switzerland	00.09%	K28911
Manaceine		Bark	Not stated	800 ppm	ZZ1095
Manacine	Alkaloid	Root Bark	Brazil Not stated	Not stated 800 ppm	W02597 ZZ1095
Mandragorine		Plant	Not stated	Not stated	ZZ1095
Mentha-28-dien-1-ol, para-	Monoterpene	Aerial Parts	Switzerland	00.05%	K28911
Myrcene	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Myristic acid	Lipid	Aerial Parts	Switzerland	Traces	K28911
Naphthalene, 1-2-3-4-tetrahydro- 1-1-6-trimethyl-	Polycyclic	Aerial Parts	Switzerland	Traces	K28911
Naphthalene, dimethyl-	Polycyclic	Aerial Parts	Switzerland	00.03%	K28911
Nerolidol	Sesquiterpene	Aerial Parts	Switzerland	00.14%	K28911
Non-2-en-4-olide, 2-3-dimethyl-	Lactone	Aerial Parts	Switzerland	Traces	K28911
Nona-2-4-dien-4-olide, 2-3-dimethyl-	Lactone	Aerial Parts	Switzerland	00.10%	K28911
Nona-trans-2-trans-4-tran-6-trien-1-al	Alkenal C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Nonadecane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911
Nonan-1-al	Alkanal C5 or More	Aerial Parts	Switzerland	00.06%	K28911
Nonane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911
Ocimene, cis-	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Ocimene, trans-	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Oct-2-trans-en-al	Alkenal C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Octa-1-cis-5-dien-3-ol	alkenol C5 or More	Aerial Parts	Switzerland	00.05%	K28911
Octa-1-trans-5-7-trien-3-ol, 3-7-dimethyl-	Monoterpene	Aerial Parts	Switzerland	00.04%	K28911
Octa-3-trans-5-cis-dien-2-one	Alkenone C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Octa-trans-3-trans-5-dien-2-one	Alkenone C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Octan-1-al	Alkanal C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Octan-3-one	Alkanone C5 or More	Aerial Parts	Switzerland	00.03%	K28911

Compound	Chemical Type	Plant Part	Plant Origin	Quantity	Ref #
Octane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911
Palmitic acid	Lipid	Aerial Parts	Switzerland	Traces	K28911
Palmitic acid methyl ester	Lipid	Aerial Parts	Switzerland	00.08%	K28911
Pent-1-en-3-one	Alkenone C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Pent-3-en-2-one, 4-methyl-	Alkenone C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Pent-4-en-1-al	Alkenal C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Pentacosane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911
Pentadecan-2-one	Alkanone C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Pentadecan-2-one, 6-10-14-trimethyl-	Alkanone C5 or More	Aerial Parts	Switzerland	00.57%	K28911
Pentadecane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911
Pentadecanoic acid	Lipid	Aerial Parts	Switzerland	Traces	K28911
Pentan-1-al	Alkanal C5 or More	Aerial Parts	Switzerland	00.06%	K28911
Pentan-1-al, 3-methyl-	Alkanal to C4	Aerial Parts	Switzerland	00.07%	K28911
Pentan-2-ol	Alkanol C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Pentan-2-one, 3-methyl-	alkanone C5 or More	Aerial Parts	Switzerland	00.03%	K28911
Phenanthrene	Polycyclic	Aerial Parts	Switzerland	Traces	K28911
Phytadiene, neo-	Diterpene	Aerial Parts	Switzerland	00.03%	K28911
Phytol	Diterpene	Aerial Parts	Switzerland	Traces	K28911
Pinoresinol diglucoside	Lignan	Root	Brazil	00.00129%	H14972
Prop-2-en-1-al, 2-methyl-	Alkanal to C4	Aerial Parts	Switzerland	00.03%	K28911
Pyrrole, 1-(3-methyl-butyl)-	Alkaloid	Aerial Parts	Switzerland	00.03%	K28911
Pyrrole, 1-methyl-	Alkaloid	Aerial Parts	Switzerland	00.03%	K28911
Pyrrole-3-carbaldehyde, 1-(3-methyl-butyl)-	Alkaloid	Aerial Parts	Switzerland	00.09%	K28911
Safranal, beta-	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Salicylate, isobutyl-	Benzenoid	Aerial Parts	Switzerland	00.07%	K28911

Compound	Chemical Type	Plant Part	Plant Origin	Quantity	Ref #
Salicylic acid 2-phenyl-ethyl ester	Benzenoid	Aerial Parts	Switzerland	Traces	K28911
Salicylic acid ethyl ester	Benzenoid	Aerial Parts	Switzerland	00.09%	K28911
Salicylic acid hexyl ester	Benzenoid	Aerial Parts	Switzerland	00.03%	K28911
Salicylic acid methyl ester	Benzenoid	Aerial Parts	Switzerland	61.49%	K28911
Salicylic acid pentyl ester	Benzenoid	Aerial Parts	Switzerland	00.07%	K28911
Scopoletin	Coumarin	Root Entire Plant Root Root Seed Rootbark Leaf + Stem	Brazil Brazil Brazil Brazil Brazil Peru Not Stated	00.0125% 00.10% 00.0033% Not stated Not stated Not stated Not stated	AY1031 A07286 L01999 T01415 A07306 H00026 M17895
Scopoletin-beta-d-xylopyranosyl(1-6)-beta-d-glucopyranoside	Coumarin	Root	Brazil	00.00258%	H14972
Scopolin	Coumarin	Leaf + Stem	Not Stated	Not stated	M17895
Sistosterol	Sterol	Root	Brazil	0.04%	AY1031
Spirosta-2-alpha-3-beta-26-triol,(5-alpha-25r)3-o-alpha-l-arabinopyranosyl(1-4)-beta-d-glucopyranosyl(1-2)-(beta-d-xylopyranosyl(1-3))-galactopyranoside	Sapogenin	Root	Brazil	00.00451%	H14972
Spirosta-3-beta-26-diol,(5-alpha-25r)- 3-o-alpha-l-arabinopyranosyl(1-4)-beta-d-glucopyranosyl(1-2)-(beta-d-xylopyranosyl(1-3))-beta-d-glucopyranosyl(1-4)-beta-d-galactopyranoside	Sapogenin	Root	Brazil	00.00107%	H14972
Stigmasterol	Sterol	Root	Brazil	0.04%	AY1031
Succinimide, 1-methyl-	Non-alkaloid Nitrogen Heterocycle	Aerial Parts	Switzerland	00.03%	K28911
Terpineol, alpha-	Monoterpene	Aerial Parts	Switzerland	00.36%	K28911
Terpineol acetate, alpha-	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Terpinolene	Monoterpene	Aerial Parts	Switzerland	00.03%	K28911
Thiophene-2-carbaldehyde, 3-propyl-	Sulfur Compound	Aerial Parts	Switzerland	00.04%	K28911

Compound	Chemical Type	Plant Part	Plant Origin	Quantity	Ref #
Tigonin, degalacto-	Sapogenin	Root	Brazil	00.00043%	H14972
Tolualdehyde	Benzenoid	Aerial Parts	Switzerland	00.07%	K28911
Toluene	Benzenoid	Aerial Parts	Switzerland	00.03%	K28911
Tricosane, n-	Alkane C5 or More	Aerial Parts	Switzerland	Traces	K28911
Xylene	Benzenoid	Aerial Parts	Switzerland	Traces	K28911

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