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Climbing the Tree of Caffeine

How to cite:

“Baumann TW and Häsler BR (2012).
The Caffeine Phylotree.
www.villacoffea.com”

March 12, 2014

Eurosids II, Malvales, Malvaceae s.l.

Cola Schott et Endl. [N° of species = 125/whereof PuA-containing ≥ 6], tropical Africa [1]. *C. nitida* and *C. acuminata*, cola nut = seed without seed coat (storage cotyledons), chewed daily, caffeine ca. 2 %, tree. Used in socio-cultural ceremonies in the area of origin [2], in our latitudes component of pharmaceutical tonics [3]. Despite great efforts to breed high-yielding varieties, the worldwide production of cola remains on a very modest level, this in disaccord with that of cola drinks!

Herrania Goudot [17/17], tropical South America incl. the isthmus [4], seeds, theacrine, 0.2 – 2 % of the defatted cocoa mass [5]. Very striking are the linear or filiform ligules of the petal up to xy cm long. In the area of origin, the sweet-sour seed pulp is eaten or the seeds serve for the preparation of a cocoa drink (e.g. *H. purpurea*, Bribri-Indios in Costa Rica; [6]). The gene pool of *Herrania* may be crucial for cocoa breeding, however, like the “wild cocoa trees” (see Xref) these species attract little attention by the chocolate community and are altogether endangered.

Theobroma L. [20/20], tropical America [7], seeds (and pulp), PuA 2–3(4.5) % of the defatted cocoa mass of *T. cacao* with theobromine as main alkaloid. The ratio out of theobromine to caffeine characterises the noblesse of the cocoa and is low (≤ 3) in the noble subspecies *cacao* and high (up to 20) in the profane *sphaerocarpum* [8] [9]. Generally, the packaging is nobler than the wrapped chocolate, because the worldwide cultivation of fine cocoa is below 5 %. Equally to *Herrania*, the seeds of the “wild cacaos” accumulate, as far as known, theacrine, however, mostly ≤ 0.5 % [5]. Worth mentioning is here *T. grandiflorum*, cupuaçu, which in Brazil is cultivated by reason of its copious and very aromatic pulp. The cupuaçu beans are used for the manufacture of the theacrine-containing “cupulate”.

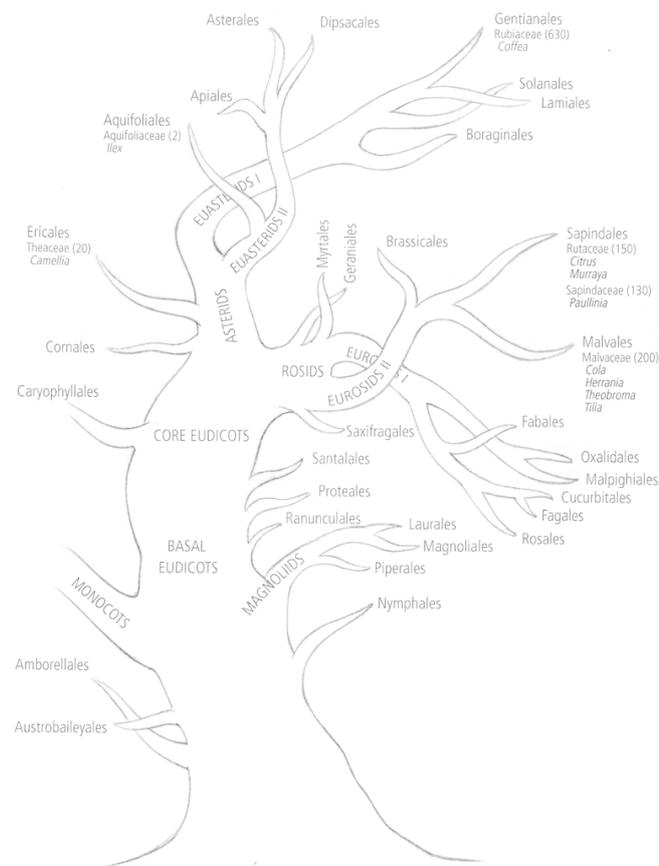


Figure 0.1 – Fig xy. Phylogenetic Tree of Angiosperms with orders, caffeine-containing families and genera. In brackets the number of genera. Illustration Beatrice Häslér, ©Verlag villacoffea

Coffea L. [103/14], Africa, *C. arabica* and *C. canephora*, arabica and robusta coffee of different provenance and varieties. Seeds, caffeine ca. 1.2 % (arabica), 2.4 % (robusta) or 0.6 % (laurina = arabica mutant). The “wild” caffeine-free species contain *inter alia* very bitter and distasteful diterpene glycosides [25]. Recently selected caffeine-free arabica plants [26] accumulate theobromine and serve for breeding of *decaffito*, that is naturally caffeine-free coffee [27]. Mature coffee fruits are consumed by several mammals and birds, which digest only the sweet “pulp” (exo- and mesocarp) and therefore excrete “pergamino” coffee in the feces. The resulting coffee is praised as the best of all, and the one produced by the Asian palm civet, *Paradoxurus hermaphroditus* is commercialised.

Asterids, Euasterids II, Aquifoliales, Aquifoliaceae

Ilex L. [400-500/6], cosmopol. but pref. in trop. and temp. Asia and America [28] [29], *I. paraguariensis*, maté tea. Leaves, caffeine around 1 %. Extremely high variability as to PuA: Caffeine- or theobromine-containing, or both, or totally alkaloid-free [30] [31]. The tea is sucked from vessels, partly very elaborate, with a tube called *bombilla*. A few wild *Ilex* species are used in ceremonies and rituals, e.g. the strongly caffeinated (more than 3%) *I. guayusa* in Peru and Ecuador, or the *I. vomitoria* with an alkaloid spectrum similar to maté in the southeast of the USA. A clustering of caffeine-containing species is recognised in the “American clade” [32] of the genus *Ilex*.

Tilia L. [23/ ≥ 1], northern hemisphere, temperate, subtropical and tropical climate [10], nectar, honey, caffeine and theophylline [11] as well as theobromine [12]. The flower parts have not yet been investigated as to PuA.

Eurosids II, Sapindales, Rutaceae

Citrus L. [20/20], presumably all “true citrus fruit trees” [13] [14] including *Poncirus*, *Fortunella*, *Microcitrus* a.s.o., anthers, pollen, and honey [15] [16], caffeine as well as theophylline, little theobromine and paraxanthine, PuA totally 0.9 % (anther), thereof ca. one third theophylline, in citrus this PuA the precursor of caffeine signifying an alternative biosynthesis route for caffeine [17]. Based upon additional (and independent) discovery of caffeine in the flower of *Murraya paniculata* (L.) Jack (orange jasmine), we may assume even a larger occurrence of this alkaloid (*i.e.* Citreae).

Eurosids II, Sapindales, Sapindaceae

Paullinia L. [194/2], lianas, tropical America [18], *P. cupana*, seeds, caffeine 3–5 %, traditionally cultivated and processed by the Indians of the Central Amazon. For stock sourcing the slightly roasted seeds are pestled and with water (and manioc) mixed to a mash, which is formed into a rod, called “bastão” or small pieces of art [19]. Toucans digest the starchy aril in the crop [20]. *P. yoco*, the rasped bark squeezed into water, caffeine 0.5–2.5%, ethnies of southern Colombia of northeast of Ecuador [20] [20].

Asterids, Ericales, Theaceae

Camellia L. [120-290/4], Southeast Asia [21] [22], *C. sinensis* with the var. *sinensis* and *assamica*, China and Assam tea of a wide range of processing. Leaves, 2–7 % caffeine, ca. 10x less theobromine, gradually decreasing from the top to the base of the plant. The variety *kucha* accumulates predominantly theacrine [23], and *C. pilophylla* only theobromine, ≤ 5 % [24]. Camellias, *i.e.* *C. japonica*, are PuA free.

Asterids, Euasterids I, Gentianales, Rubiaceae

Bibliography

- [1] Pan AD and Jacobs BF. The earliest record of the genus *Cola* (Malvaceae *sensu lato*: Sterculioideae) from the Late Oligocene (28–27 Ma) of Ethiopia and leaf characteristics within the genus. *Plant Syst Evol*, 283(3-4):247–262, 2009. (document)
- [2] Weckerle CS, Timbul V, and Blumenshine PM. *Plants, Health and Healing: On the Interface of Ethnobotany and Medical Anthropology*, chapter Medicinal, stimulant and ritual plant use: An ethnobotany of caffeine-containing plants, pages 262–301. Berghahn Books, Oxford, 2010. (document)
- [3] Seitz R and Kraus L. *Hagers Handbuch der Pharmazeutischen Praxis*, volume 4, Drogen A-D, chapter Cola, pages 940–946. Springer-Verlag, Berlin, 1992. (document)
- [4] Schultes RE. A synopsis of the genus *Herrania*. *Journal Arnold Arboretum*, 39:216–295, 1958. (document)
- [5] Hammerstone JF, Romanczyk LJ Jr L, and Aitken WM. Purine alkaloid distribution within *Herrania* and *Theobroma*. *Phytochemistry*, 35(5):1237–1240, 1994. (document)
- [6] Pittier H. New or noteworthy plants from Colombia and Central America—4. *Contr. US Nat. Herb.*, 18(2):69–86, 1914. (document)
- [7] Cuatrecasas J. Cacao and its allies. A taxonomic revision of the genus *Theobroma*. *Contrib. U.S. National Herb.*, 35(6):379–614, 1964. (document)
- [8] Asamoia Y and Wurziger J. Coffeingehalt in Kakaobohnen. *Gordian*, 76:138–139, 1976. (document)
- [9] Sotelo A and Alvarez RG. Chemical composition of wild *Theobroma* species and their comparison to the cacao bean. *J. Agric. Food Chem.*, 39:1940–1943, 1991. war Dissprüfungspaper. (document)
- [10] Muir N. A survey of the genus *Tilia*. *Plantsman*, 5:206–242, 1984. (document)
- [11] Naef R, Jaquier A, Velluz A, and Bachofen B. From the linden flower to linden honey – Volatile constituents of linden nectar, the extract of bee-stomach and ripe honey. *Chemistry & Biodiversity*, 1(12):1870–1879, 2004. (document)
- [12] Horzic D, Komes D, Belscak A, Kovacevic Ganic K, Ivekovic D, and Karlovic D. The composition of polyphenols and methylxanthines in teas and herbal infusions. *Food Chemistry*, 115(2):441–448, JUL 15 2009. (document)
- [13] Samuel R, Ehrendorfer F, Chase MW, and Greger H. Phylogenetic analyses of Aurantioideae (Rutaceae) based on non-coding plastid DNA sequences and phytochemical features. *Plant Biology*, 3(1):77–87, 2001. (document)
- [14] Mabberley DJ. *Citrus* (Rutaceae): A review of recent advances in etymology, systematics and medical applications. *Blumea*, 49(2-3):481–498, 2004. (document)
- [15] Stewart I. Identification of caffeine in citrus flowers and leaves. *Journal of Agricultural and Food Chemistry*, 33(6):1163–1165, 1985. (document)
- [16] Kretschmar JA and Baumann TW. Caffeine in *Citrus* flowers. *Phytochemistry*, 52:19–23, 1999. (document)
- [17] Weckerle CS, Stutz MA, and Baumann TW. Purine alkaloids in *Paullinia*. *Phytochemistry*, 64(3):735–742, 2003. (document)
- [18] Weckerle CS and Rutishauser R. Gynoecium, fruit and seed structure of Paullinieae (Sapindaceae). *Botanical Journal of the Linnean Society*, 147(2):159–189, FEB 2005. (document)
- [19] Henman AR. Guaraná (*Paullinia cupana* var. *sorbilis*): Ecological and social perspectives on an economic plant of the central Amazon basin. *J. Ethnopharmacol.*, 6:311–338, 1982. (document)
- [20] Baumann TW, Schulthess BH, and Hänni K. Guaraná (*Paullinia cupana*) rewards seed dispersers without intoxicating them by caffeine. *Phytochemistry*, 39(5):1063–1070, 1995. (document)
- [21] Prince LM. A brief nomenclatural review of the genera and tribes in Theaceae. *Aliso*, 24:105–121, 2007. (document)
- [22] Vijayan K, Zhang WJ, and Tsou CH. Molecular taxonomy of *Camellia* (Theaceae) inferred from nrITS sequences. *American Journal of Botany*, 96(7):1348–1360, 2009. (document)
- [23] Lu JL, DM Wang, Shi XG, Yang DP, Zheng XQ, and Ye CX. Determination of purine alkaloids and catechins in different parts of *Camellia assamica* var. *kucha* by HPLC–DAD/ESI–MS/MS. *Journal of the Science of Food and Agriculture*, 89(12):2024–2029, 2009. (document)
- [24] Yang XR, Ye CX, Xu JK, and Jiang YM. Simultaneous analysis of purine alkaloids and catechins in *Camellia sinensis*, *Camellia ptilophylla* and *Camellia assamica* var. *kucha* by HPLC. *Food Chemistry*, 100(3):1132–1136, 2007. (document)

- [25] Prewo R, Guggisberg A, Lorenzi-Riatsch A, Baumann TW, and Wettstein-Bättig M. Crystal structure of mozambioside, a diterpene glycoside of *Coffea pseudozanguebariae*. *Phytochemistry*, 29(3):990–992, 1990. (document)
- [26] Silvarolla MB, Mazzafera P, and Fazuoli LC. A naturally decaffeinated arabica coffee. *Nature*, 429(6994):826–826, 2004. (document)
- [27] Mazzafera P, Baumann TW, Shimizu MM, and Silvarolla MB. *Decaf* and the steeplechase towards *Decaffito*—the coffee from caffeine-free Arabica plants. *Tropical Plant Biology*, 2(2):263–276, 2009. (document)
- [28] Cuenoud P, Martinez MAD, Loizeau PA, Spichiger R, Andrews S, and JF Manen. Molecular phylogeny and biogeography of the genus *Ilex* L. (Aquifoliaceae). *Annals of Botany*, 85(1):111–122, 2000. (document)
- [29] Galle FC. *Hollies. The genus Ilex*. Timber Press, Portland, Oregon, 1997. (document)
- [30] Zographos VA. *Purinalkaloide in der Gattung Ilex – eine taxonomische Hilfe?* Master thesis, University of Zurich, 1998. (document)
- [31] Athayde ML, Coelho GC, and Schenkel EP. Populational diversity on methylxanthines content of mate (*Ilex paraguariensis* A. St.-Hil., Aquifoliaceae). *Latin American Journal of Pharmacy*, 26(2):275–279, 2007. (document)
- [32] Selbach-Schnadelbach A, Smith Cavalli S, Manen JF, Coelho GC, and Teixeira De Souza-Chies T. New information for *Ilex* phylogenetics based on the plastid psbA-trnH intergenic spacer (Aquifoliaceae). *Botanical Journal of the Linnean Society*, 159(1):182–193, 2009. (document)