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Floral Flavonoids and the Systematics of *Simsia* (Asteraceae: Heliantheae)

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ABSTRACT. Data from floral flavonoid chemistry of *Simsia* are not of widespread use in analyzing interspecific relationships but bear on a few problems within the genus. Most members of the "*S. fruticulosa* group" share a relatively simple floral flavonoid profile based on quercetin glycosides. In the "*S. amplexicaulis* group", which is characterized by flavone glycosides in addition to quercetin glycosides, the presence of apigenin 7-glucoside links *S. lagascaeformis* and *S. eurylepis*, and the presence of coreopsin/sulfurein unites *S. foetida*, *S. grandiflora*, *S. guatemalensis*, *S. megacephala*, and *S. panamensis*. The presence of coreopsin/sulfurein in *S. chaseae* provides a chemical trait to link it to *S. foetida*, one of the putative parental species in the hypothesis of diploid hybrid speciation that has been proposed for its origin. At the generic level, the occurrence of anthochlors links *Simsia* to *Viguiera* and related genera. Among these genera it appears that in floral flavonoids *Simsia* is characterized by a relatively distinctive compound, quercetin 3-glucuronide.

Simsia Persoon is a genus of 18 species and seven varieties divided into two sections (Spooner 1987a), here referred to as the "*S. fruticulosa* group" and the "*S. amplexicaulis* group". The genus is entirely New World in distribution, extending from the southwestern United States to Argentina with one additional taxon endemic to Jamaica (Robinson and Brettell 1972; Spooner 1987a). *Simsia* is distinguished from *Viguiera* Kunth, the most closely related genus, by the pappus of two awns without the presence of intermediate squamellae, and by the achene which is generally flattened with a thin outer margin. *Viguiera* has biconvex achenes and a pappus usually of two awns that also includes squamellae. Features of the style branches have also been used to link *Simsia* to *Helianthus* L. (Robinson 1979); however, *Helianthus* differs by having a deciduous rather than persistent pappus. Together with a few other elements, these genera form a clearly related but imperfectly distinguished group that forms the bulk of subtribe Helianthinae (Robinson 1981).

There are two general problem areas in *Simsia* to which we wanted to apply floral flavonoid data. One involves species relationships in the genus. There are few morphological characters that clearly link large segments of the genus (Spooner 1987a), and hence the presence of diagnostic chemical features would be of great value. We were also interested in detecting characters by which to analyze possible hybridization in *Simsia*.

The second major problem involves the delimitation between *Simsia* and the closely related *Viguiera*. Several of the groups of *Viguiera* that previously have been examined have distinctive floral flavonoids (Rieseberg and Schilling 1985; Schilling et al. 1988; Schilling, unpubl. data), and we hoped to identify distinctive features in *Simsia* which might be used to clarify its generic relationships.

MATERIALS AND METHODS

Flowering heads of *Simsia* were collected from natural populations (table 1), representing all taxa of the genus except for *S. tenuis* (Fern.) S. F. Blake and *S. jamaicensis* S. F. Blake. Flavonoid procedures generally followed those of Mabry et al. (1970). Methanolic extracts of dried heads were concentrated and spotted on Whatman 3MM chromatography paper. Chromatograms were developed in TBA (3:1:1 t-butanol : acetic acid : water) and 15% acetic acid. Spots visualized with UV light were cut from chromatograms and extracted with methanol. Final purification utilized column chromatography on

Sephadex LH-20 in methanol (Markham 1982). Identification was based on color under UV light, UV spectral data, and cochromatography with authentic compounds identified from previous studies of *Helianthus* and *Viguiera*.

RESULTS AND DISCUSSION

The systematic distribution of flavonoids isolated from *Simsia* flowering heads is shown in table 2. Several species of *Simsia* lack flavonoids in ray flowers, and one species, *S. eurylepis* (see table 2 for authors), lacks ray flowers completely. For this reason, whole head extracts were used for flavonoid analysis of all species.

Compounds present in *Simsia* flowering heads include flavonols, flavones, and anthochlors (table 2). The 3-glucoside of quercetin occurs in all *Simsia* species but is such a common compound in general that its presence is of no taxonomic significance. The 3-glucuronide is almost as widespread in the genus, but it is a much rarer compound in plants in general, and it has not previously been reported to occur in any closely related genus. The 7-glucoside has a sporadic occurrence throughout the genus. Flavone glycosides occur exclusively in the "*S. amplexicaulis* group" and appear to characterize it within the genus. Anthochlor glycosides occur in relatively few species of *Simsia*. The relatively limited amount of interspecific flavonoid variation is in agreement with data from morphology and crossing studies (Spooner 1987a) that suggest that *Simsia* is of relatively recent origin.

With the exception of *S. ghiesbreghtii*, all the species of the "*S. fruticulosa* group" have similar floral flavonoid profiles (table 2). Several species lack ray flavonoids, and compounds are all quercetin glycosides.

Simsia ghiesbreghtii is exceptional within the "*S. fruticulosa* group" in containing anthochlors (table 2), and it also is unusual in other respects. This species is variable for several of the characters that are used to separate *Simsia* and *Viguiera*; in particular, characters of the achenes and pappus. Some populations have the typical Simsioid flattened achenes that lack pappus squamellae, but others have biconvex achenes that may have several squamellae. Hence the presence of anthochlors, and particularly the rarely observed anthochlor pair marein/maritimein, in *S. ghiesbreghtii* is of interest. The only other related plant that is known to exhibit these compounds is *Viguiera dentata* (Rieseberg and Schilling 1985); it is not clear whether this represents homoplasy or is an indication that these taxa have a close phyletic relationship.

Several species of the "*S. amplexicaulis* group" have distinctive floral flavonoid traits (table 2). The shared occurrence of apigenin 7-glucoside in *S. lagascaeformis* and *S. eurylepis* provides a similarity to support the proposed relationship of these species based on morphological data (Spooner 1987a). The occurrence of the anthochlor pair coreopsin/sulfurein provides a unifying trait for the species (*S. foetida, S. grandiflora, S. guatemalensis, S. megacephala,* and *S. panamensis*) that are considered as varieties of *S. foetida* (Spooner 1987a). The floral flavonoid profile of *S. chaseae* is identical to certain of these taxa (table 2), which is consistent with the proposed origin of *S. chaseae* as a derivative of diploid hybridization between *S. eurylepis* and *S. foetida* s.l. (Spooner 1987b). Spooner (1987a) has further cited evidence from morphology

TABLE 1. *Simsia* samples analyzed for floral flavonoids. Vouchers deposited at OS. Collector abbreviations: B—A. Burgos; D—O. R. Dorado R.; E—E. E. Schilling; G—J. Guevara; V—J. L. Villaseñor R.; S—D. M. Spooner.

S. amplexicaulis—MÉXICO, Chihuahua: *S&E 2453, S. annectens*—MÉXICO, Guerrero: *S 2845, S. calva*—MÉXICO, Nuevo León: *S 2482, S. chaseae*—MÉXICO, Quintana Roo: *S 2811*; Yucatan: *S 2803, S. dombeyana*—ECUADOR, Guayas: *S 2908, S. eurylepis*—MÉXICO, Nuevo León; *S 2481*; Veracruz: *S 2882, S. foetida*—MÉXICO, Puebla: *S&D 2637, S. fruticulosa*—COLOMBIA, Cundinamarca: *S&G 2921*; Huila: *S&G 2923, S. ghiesbrightii*—MÉXICO, Chiapas: *S 2681*; GUATEMALA, Quezaltenango: *S&D 2695*; San Marcos: *S&D 2674, S. grandiflora*—HONDURAS, El Valle: *S&D 2699, S. grayi*—MÉXICO, México: *S&V 2562, S. guatemalensis*—MÉXICO, Chiapas: *S 2769*; GUATEMALA, Guatemala: *S&D 2693, S. holwayi*—GUATEMALA, El Progreso: *S&D 2746*; Guatemala: *S&D 2690, S. lagascaeformis*—MÉXICO, Guerrero: *S&B 2603, 2606*; Jalisco: *S&V 2489*; Morelos: *S&B 2600*; Oaxaca: *S&D 2656, S. megacephala*—MÉXICO, Oaxaca: *S&D 2667, S. molinae*—NICARAGUA, Estelí: *S&D 2701*; Managua: *S&D 2714, S.* sp. nov. "A"—COSTA RICA, Guanacaste: *S 2900, S.* sp. nov. "B"—MÉXICO, Oaxaca: *S 2816, S. panamensis*—PANAMA, Panama: *S 2902, S. sanguinea*—MÉXICO, Jalisco: *S&V 2495*; México: *S&V 2567*; GUATEMALA, Sololá: *S&D 2681, S. setosa*—MÉXICO, Nayarit: *S&V 2528, S. steyermarkii*—GUATEMALA, Baja Verapaz: *S&D 2748, S. triloba*—MÉXICO, Oaxaca: *S&D 2641a, 2649b.*

TABLE 2. *Simsia* flora flavonoids. Ray compounds: +, present in ray flowers; −, absent in ray flowers; abs, ray flowers lacking. Compounds. 1 = quercetin 3-glucoside, 2 = quercetin 3-glucuronide, 3 = quercetin 7-glucoside, 4 = apigenin 7-glucoside, 5 = luteolin 7-glucoside, 6 = coreopsin/sulfurein, 7 = marein/maritimein.

Taxon	N	Ray compounds	Compounds 1	2	3	4	5	6	7
"*S. fruticulosa* group"									
S. annectens S. F. Blake	1	+	+	+	+	−	−	−	−
S. calva (A. Gray & Engelm.) A. Gray	1	−	+	−	−	−	−	−	−
S. fruticulosa (Spreng.) S. F. Blake	2	−	+	+	−	−	−	−	−
S. ghiesbreghtii (A. Gray) S. F. Blake	3	+	+	−	−	−	−	+	+
S. grayi Sch.Bip. ex S. F. Blake	1	+	+	+	−	−	−	−	−
S. holwayi S. F. Blake	2	+	+	+	+	−	−	−	−
S. molinae H. Robinson & Brettell	2	−	+	+	+	−	−	−	−
S. sanguinea A. Gray	3	−	+	+	+	−	−	−	−
S. setosa S. F. Blake	1	−	+	+	−	−	−	−	−
S. sp. nov. "A", *Spooner 2900*	1	−	+	+	−	−	−	−	−
S. sp. nov. "B", *Spooner 2816*	1	−	+	+	+	−	−	−	−
S. steyermarkii H. Robinson & Brettell	1	−	+	+	+	−	−	−	−
S. triloba S. F. Blake	2	+	+	+	+	−	−	−	−
"*S. amplexicaulis* group"									
S. amplexicaulis (Cav.) Persoon	1	+	+	+	−	−	+	−	−
S. chaseae (Millsp.) S. F. Blake	2	+	+	+	−	−	+	+	−
S. dombeyana DC.	1	−	+	+	−	−	−	+	−
S. eurylepis S. F. Blake	2	abs	+	+	−	+	+	−	−
S. foetida (Cav.) S. F. Blake	1	+	+	+	+	−	+	+	−
S. grandiflora Benth. ex Oerst.	1	+	+	−	+	−	+	+	−
S. guatemalensis H. Robinson & Brettell	2	+	+	+	−	−	+	+	−
S. lagascaeformis DC.	5	+	+	+	−	+	+	−	−
S. megacephala Sch.Bip. ex S. F. Blake	1	+	+	+	−	−	+	+	−
S. panamensis H. Robinson & Brettell	1	+	+	−	−	−	+	+	−

and breeding systems to suggest that *S. dombeyana* was derived from *S. chaseae.* Flavonoid data provide support for this in the shared occurrence of coreopsin/sulfurein in these species (table 2).

At the generic level, the presence of anthochlors provides another character to place *Simsia* within the group of genera close to *Viguiera.* Among this group of genera, anthochlors have now been reported for *Tithonia* Desf. ex A. L. Juss. (La Duke 1982), *Helianthus* (Harborne and Smith 1978; Schilling 1982; Schilling and Mabry 1981; Schilling et al. 1987), *Heliomeris* Nutt. (Shimokoriyama and Geissman 1960), and *Viguiera* (Rieseberg and Schilling 1985; Schilling and Panero 1988; Schilling et al. 1988), and also occur in *Helianthopsis* H. Robinson (unpubl. data). As pointed out by Crawford and Stuessy (1981), anthochlors occur in tribe Heliantheae only in subtribe Coreopsidinae and in *Viguiera* and related genera.

Simsia is characterized by a distinctive floral flavonoid, quercetin 3-glucuronide, a compound that has not previously been reported to occur among closely related genera. The absence of this compound from *Helianthus,* which has been surveyed fairly comprehensively, is evidence of a lack of close relationship between these genera. In contrast, we recently have detected quercetin 3-glucuronide in floral extracts of some species of *Viguiera* ser. *Grammatoglossae* S. F. Blake that have been proposed to be closely related to *Simsia* based on morphology. This suggests that the presence of quercetin 3-glucuronide will not be a diagnostic feature for *Simsia,* but that it may help to clarify its relationship to *Viguiera.*

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