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Solanum Chemosystematic Aspects: Analysis of Mixed Pathway (Acetate/Shikimate) Special Metabolites

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Abstract *Solanum* L. is a large, diverse and important Solanaceae genus, which taxonomy and infrageneric relationships are still unresolved, as well as its evolutionary history. Biosynthesized from the mixed pathway (acetate/shikimate) and considered good systematic markers, flavonoids are widely distributed among plant species, as also in *Solanum*. Through analysis of flavonoid chemical data, this work aims to study evolutionary polarizations and contribute towards the comprehension of species phylogenetic relationships in the genus. The chemosystematic analysis was conducted through calculation of flavonoids chemical parameters and employing multivariate statistical analysis (factor analysis). Chemical data survey led to the identification of 479 metabolites from the mixed pathway. The results obtained demonstrate *Solanum* species prefer to biosynthesize hydroxylflavonoids. However, when oxy-groups are protected, choose O-glycosylflavonoids rather than O-methylflavonoids. The chemometric analysis showed derivation of eight *Leptostemonum* species, clearly separated from the rest of *Solanum* due to O-methylation. This feature suggests a possible advancement of *Leptostemonum* species. At last, considering this preliminary analysis, it was possible to identify remarkable trends in flavonoid evolution in *Solanum* species.

Keywords *Solanum*, Solanaceae, Chemosystematic, Mixed Pathway, Flavonoids

1. Introduction

Solanum L. is the largest Solanaceae genus and comprises about 1,400 species with worldwide distribution [1, 2]. Its species possess great social and economic value as food, like potato (*S. tuberosum*) and tomato (*S. lycopersicum*), as also as medicine, such as jurubeba (*S. paniculatum*).

Over time, *Solanum* species have been studied and classified by many taxonomists based on morphological and anatomical characteristics. Dunal (1813; 1852), D'Arcy (1972; 1991), Nee (1999) and Hunziker (2001) published the main *Solanum* works [3-8], being D'Arcy's classification system (1972) the most used and accepted worldwide.

The advent of molecular phylogeny contributed towards a better understanding of *Solanum* taxonomy. From the 90's, a series of studies conducted using this approach [9-12] resulted in an infrageneric classification of *Solanum* in thirteen subspecies group: *African non-spiny*, *Archaesolanum*, *Brevantherum*, *Cyphomandra*, *Dulcamaroid*, *Geminata*, *Leptostemonum*, *Morelloid*, *Normania*, *Potato*, *Regmandra*, *Thelopodium* and *Wendlandii-Allophyllum* [12].

While *Solanum* genus presents great morphological diversity, its species exhibit uniform aspects, like pentamerous perianth and androceus, connivent stamens and poricidal anther dehiscence. *Solanum* also has species showing different habit types, from herbs to small trees, shrubs and vines [13, 14]. Due to the size and morphological diversity found in the genus, problems concerning taxonomical classification are not well comprehended yet.

Chemical evolution displayed in *Solanum* results from an evolutionary channeling manifested by gradients related to morphology and metabolism. Although recently plant systematics has elucidated *Solanum* taxonomy, many controversies are still unresolved [9-12].

In this study, special metabolites from the mixed pathway were used as systematic markers to evaluate *Solanum* genus diversification. Thus, these chemical data can be exploited based on the assumption flavonoids are good systematic markers, since its biosynthetic relationships and evolutionary scheme are well known [15], allowing to distinguish primitive metabolites from more advanced ones in angiosperms.

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This work aims to study *Solanum* evolutionary polarizations through analysis of its chemomarkers occurrence pattern. It is intended to help in a better understanding of species phylogenetic relationships in the genus, employing chemosystematic methodology approach.

2. Materials and Methods

2.1. Chemosystematic Methodology

Chemical data research was performed on *Scifinder* database covering papers published from 1902 to 2016. Survey was conducted using as keywords the name of species belonging to each *Solanum* subgenus, following Weese and Bohs (2007) phylogenetic classification [12].

Metabolites biosynthesized by the mixed pathway were classified according to their flavonoid class, as well as were counted the occurrence number (ON).

Chemosystematics analysis was conducted as described by Gottlieb et al (1996) methodology [16]. This approach is based on the calculation of chemical parameters for each metabolite, such as: evolutionary advancement oxidation (EA_O) and skeleton specialization index (EA_E); flavonoid protection and unprotection indices: EA_G (O-glycosylation), EA_M (O-methylation), EA_{TP} (O-total protection) and EA_{TU} (O-total unprotection).

While, oxidation (O) and skeleton specialization (E) indices were determined based on the following equations 1 and 2:

$$O = \frac{(x - h)}{n} \quad (1)$$

$$E = \frac{(q + f + c + u)}{n} \quad (2)$$

Where:

x = number of C – heteroatom bonds;

h = number of C – H bonds;

n = number of carbon atoms in the molecular skeleton;

q = number of broken C – C bonds in relation to a precursor;

f = number of formed C – C bonds in relation to a same precursor;

c = number of cyclic systems formed involving heteroatoms in relation to a same precursor;

u = number of carbonic additional units in relation to a precursor;

Evolutionary advancement oxidation (EA_O) and skeleton specialization (EA_E) indices were obtained by the following equations 3 and 4, respectively:

$$EA_O = \frac{\sum O}{ON} \quad (3)$$

$$EA_E = \frac{\sum E}{ON} \quad (4)$$

The phenolic substitution pattern in flavonoids was also investigated by means of evolutionary advancement indices, such as EA_G (O-glycosylation), EA_M (O-methylation), EA_{TP} (O-total protection) and EA_{TU} (O-total unprotection), as shown in equations 5, 6, 7 and 8:

$$EA_G = \frac{\sum GI}{ON} \quad (5)$$

$$EA_M = \frac{\sum MI}{ON} \quad (6)$$

$$EA_{TP} = \frac{\sum TP}{ON} \quad (7)$$

$$EA_{TU} = \frac{\sum TU}{ON} \quad (8)$$

Where:

ON: occurrence number;

GI: O-glycosyl group number/ total oxy-group number;

MI: O-methyl group number/ total oxy-group number;

TP: oxy-group protected number/ total oxy-group number;

TU: oxy-group unprotected number/ total oxy-group number;

The relation between flavones (fo) and flavonols (fl) bioproduction was calculated for each *Solanum* subgenus [17]. This parameter consists in an important factor to establish morphological and chemical diversity relationship:

$$\frac{fo}{fl} = \frac{\text{flavone ON}}{\text{flavonol ON}} \quad (9)$$

2.2. Multivariate Analysis

Multivariate statistical analysis was performed using factor analysis technique. Software used for data treatment was Statistica® 12 for Windows.

3. Results and Discussion

3.1. *Solanum* Chemical Profile

Bibliographic survey of *Solanum* chemical data led to 923 papers. 479 metabolites from the mixed pathway were identified. The distribution in nine *Solanum* subgenera resulted in the following occurrence number: *Leptostemonum* (ON=180); *Brevantherum* (ON=20); *Geminata* (ON=7); *Cyphomandra* (ON=57); *Morelloid* (ON=50); *Dulcamaroid* (ON=52); *Potato* (ON=106); *Archaesolanum* (ON=4) and *African non-spiny* (ON=3). *Regmandra, Normania, Thelopodium and Wendlandii-Allophyllum* subgenera do not have literature report of mixed pathway metabolites.

Among *Solanum* major metabolites, it can be highlighted the predominant flavonol occurrence in nearly all subgenera, as in *Leptostemonum* (ON=132), *Potato* (ON=64), *Dulcamaroid* (ON=27), *Morelloid* (ON=20), *Brevantherum* (ON=19), *Geminata* (ON=5) e *Archaesolanum* (ON=4). Species belonging to *Cyphomandra* presents flavonol (ON=21), but anthocyanidin predominates (ON=31). No flavonol reports were found in *African non-spiny* subgenus, showing only anthocyanidin presence (ON=3).

Regarding structural diversity of *Solanum* metabolites from the mixed pathway, it is noted the presence of few relevant flavonoidic classes, such as anthocyanidins (ON=82), catechins (ON=19), chalcones (ON=6),

coumestans (ON=4), dihydroflavonols (ON=2), flavones (ON=29), flavonols (ON=292), flavanones (ON=24), isoflavonoids (ON=20) and stilbenes (ON=1). Table 1 summarizes the occurrence number of flavonoidic classes of each species. This feature demonstrates flavonoids bioproduction is still in transition in *Solanum* genus.

However, due to the mixed pathway homology, chemical similarity between species belonging to the same subgenus is supported by flavonoid structural variation and even by analogous evolutionary aspects [18].

The study reveals that flavonoidic structural diversification occurs simultaneously and is in an intermediary phase in the genus. *Solanum* flavone/flavonol ratio (0.07) shows flavonols represents the most important mixed pathway subclass in all *Solanum* subgenera analyzed for this parameter. Flavone/flavonol ratio of *Solanum* subgenera are, as follows: *Leptostemonum* (0.12); *Dulcamaroid* (0.11); *Morelloid* (0.10); *Potato* (0.09); *Brevantherum* (0.05); *Cyphomandra* (0.05); *Archaesolanum* (0); *Geminata* (0).

Higher prevalence of flavonols instead of flavones is a significant correlation parameter between morphological and chemical features. This aspect demonstrates a primitive character in the flavonoid chemistry of *Solanum*.

Table 1. Occurrence number (ON) of mixed pathway metabolites of *Solanum* species classified according to micromolecular category; Codes: ANT (anthocyanidin), CAT (catechin), CHA (chalcone), COU (coumestan), DIH (dihydroflavonol), FLAVA (flavanone), FLON (flavone), FLOL (flavonol), IFL (isoflavonoid), STI (stilbene). Data collected on *SciFinder* database covering papers from 1902 to 2016

Code	Species	ANT	CAT	CHA	COU	DIH	FLAVA	FLON	FLOL	IFL	STI
AF	*S. guineense*	3									
A2	*S. laciniatum*								4		
L4	*S. aethiopicum*								1		
L5	*S. agrarium*								2		
L7	*S. angustifolium*								2		
L8	*S. anguivi*								2		
L19	*S. citrullifolium*								3		
L20	*S. coagulans*							1	6		
L24	*S. elaeagnifolium*					1		2	19		
L26	*S. glabratum*							1	2		
L28	*S. grayi*							2			
L30	*S. heterodoxum*								2		
L32	*S. incanum*							4	12		
L34	*S. jabrense*							1	14		
L38	*S. macrocarpon*								2		
L41	*S. melongena*	22	1						10		
L42	*S. palinacanthum*								1		
L43	*S. paludosum*							2	7	1	
L44	*S. paniculatum*								2		
L45	*S. paraibanum*								5		
L47	*S. quitoense*								4		
L48	*S. rhytidoandrum*							1	5		
L50	*S. rostratum*								4		
L52	*S. schimperianum*								7		
L53	*S. sessiliflorum*						1				
L54	*S. sisymbrifolium*	1							2		
L58	*S. tenuipes*								3		
L59	*S. torvum*							2	15	2	
L62	*S. viarum*			2			1				
B2	*S. asperum*								3		
B4	*S. cernuum*								13		
B5	*S. erianthum*							1	3		

Code	Species	ANT	CAT	CHA	COU	DIH	FLAVA	FLON	FLOL	IFL	STI
G10	*S. oblongifolium*						1		1		
G13	*S. spirale*		1						1		
G11	*S. pseudocapsicum*								2		
C2	*S. betaceum*	31	3			1		1	9		
C3	*S. corymbiflorum*								1		
C4	*S. glaucophyllum*								11		
D2	*S. crispum*		1						8		
D3	*S. dulcamara*								7		
D6	*S. lyratum*				4			3	10	17	
D10	*S. valdiviense*								2		
M1	*S. americanum*	2							1		1
M3	*S. chenopodioides*								1		
M5	*S. nigrum*	6	8				3	2	14		
M8	*S. retroflexum*								1		
M10	*S. scabrum*	8							2		
M13	*S. villosum*								1		
P1	*S. acaule*	3	2				2		2		
P3	*S. berthaultii*	3	2				2		2		
P5	*S. cardiophyllum*		1								
P13	*S. demissum*								1		
P16	*S. habrochaites*						1		8		
P20	*S. jamesii*								2		
P29	*S. muricatum*						1		3		
P31	*S. neorickii*								3		
P35	*S. pimpinellifolium*								1		
P36	*S. pinnatisectum*								2		
P41	*S. stoloniferum*							1	1		
P25	*S. lycopersicum*	3		4			12	5	39		
P43	*S. tuberosum*	46	2					1	14		

Primitiveness is confirmed by two parameters obtained for the Solanaceae family: Sporne (IS=68) and Herbaceousness (IH=50) indices [15, 17, 19]. *Solanum* shows a preference in flavonol bioproduction that may indicate a more primitive taxon positioning [20], according to Bate-Smith (1962).

Concerning phenolic protection and analyzing chemical modulatory indices, as detailed in table 2, it is clearly noted the trend for unprotection of flavonoidic hydroxyls in *Solanum* species.

However, it is observed a derivation of some species belonging to the *Leptostemonum* subgenus from the rest of *Solanum*. This behavior is noted in eight *Leptostemonum* species (L19, L26, L30, L34, L43, L45, L48, L58), which exhibits more than 50% of O-methylation in flavonoids. When protected, others species shows O-glycosylation protection preference and in some cases, associates both O-glycosylation and O-methylation protection.

Solanum flavonoidic chemistry is dominated by unprotected flavonoids. Although being a basal feature, this analysis reveals that the genus is in transition due to the slight presence of different oxygenated groups protection patterns. However, it is worth noting O-glycosylation and O-methylation are protection mechanisms elaborated by *Solanum* species and represent final stages in flavonoid biosynthesis [21].

Thus, hydroxylflavonoids bioproduction and the absence of flavones could indicate group primitiveness [15, 20]. However, micromolecules biosynthesis deriving from acid acetic pathway shows to predominate in *Solanum* [22].

Regarding evolutionary advancement skeleton specialization index (EA_E) it is verified species have low values that do not differentiate each other. Only AF (EA_E=1.6889) is far from the rest of *Solanum*, due to the presence of acylated and glycosylated anthocyanidin in this taxon.

Solanum species presents extremely low EA_O index values, which is in agreement with flavonoids oxygenation patterns found in the genus. Its flavonols demonstrates ring B [(3',4'), (3',4',5') and (5,6)] oxidation patterns, besides [(5,7) and (5,7,8)] in ring A. Thus, *Solanum* shows a poor oxidative evolutionary advancement, which is characteristic of basal angiosperms, such as high index of hydroxylflavonoids.

EAO index and phenolic protection correlation seems to indicate evolutionary biosynthetic trends of species based upon gradual replacement of flavonoids less oxygenated and glycosylated to more oxygenated metabolites and methylated.

3.2. Chemosystematic Data: Chemometric Analysis

Factor analysis of chemosystematic parameters of *Solanum* species assigned to Factor 1 were O-methylation (EA_M), O-Total Protection (EA_{TP}) and Total Unprotection (EA_{TU}). To Factor 2 were attributed O-glycosylation (EA_G) and EA_E variables. Thus, bidimensional diagram (Figure 1) represents factor analysis of 62 *Solanum* species, disclosing a great dispersal between them. Analysis shows Factor 1 variables causes a high species dispersal and separate them in four groups.

First group is represented by eight *Leptostemonum* species L19, L26, L30, L34, L43, L45, L48, L58 clearly separated from the others. These *Solanum* species exhibit more than a half of their flavonoids oxy-groups highly protected. Besides, hydroxyls are protected exclusively by O-methylation mechanisms, as can be seen in data table (Table 1).

Next, second group comprises A2, M10, B2, B5, P43, M1, P16, L52, L28, L5, G10, D6 species, characterized by double protection mechanisms. All species of this group have flavonoids protected simultaneously by O-methylation and O-glycosylation. Indices related to each species are summarized in table 2.

Whereas, species B4, C2, C3, C4, D2, D3, D10, G4, G11, G13, L4, L7, L8, L20, L24, L32, L38, L41, L42, L44, L47, L50, L53, L54, L59, L62, M3, M5, M8, M13, P1, P3, P5, P13, P20, P25, P29, P31, P35, P36, P41 are included in the third group. This species set presents mostly unprotected flavonoids. When protected, it shows preference by O-glycosylation, as can be observed in table 2.

AF is distant from other *Solanum* species, forming a separated group due to parameters of Factor 2 (EA_G and EA_E).

Evolutionary advancement specialization index (AF EA_E: 1.6889) is determinant, being the highest of all *Solanum* species, due to acylated and glycosylated anthocyanidin presence in this subgenus.

As can be seen in figure 1, factor 1 contributed to differentiate groups 1, 2 and 3 according to the phenolic/oxy-groups protection parameters (AE_{OMet}, AE_{TP}, AE_{TU}). While factor 2 is important in separation of the group represented by AF from other *Solanum* species, due to AE_{OGly} parameter and the advancement skeleton specialization index (EA_E). Contributions of each variable to factors 1 and 2 are detailed in table 3.

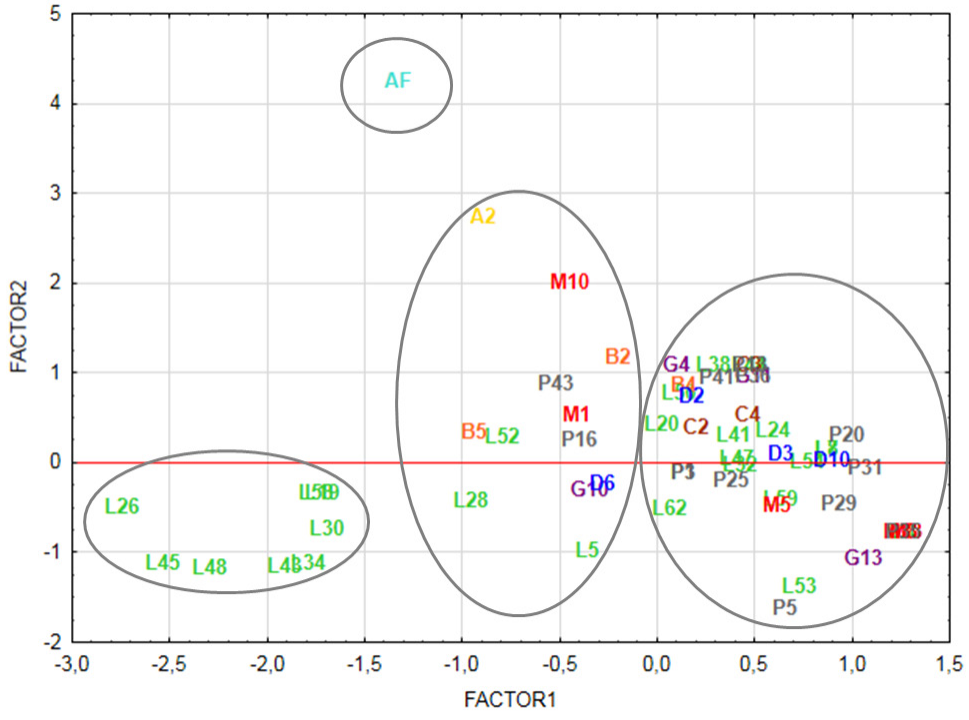

Figure 1. Bidimensional diagram representing factor analysis of parameters of mixed pathway metabolites of 62 *Solanum* species; Factor 1 (EA_M, EA_{TP} and EA_{TU}) and Factor 2 (EA_G and EA_E)

Table 2. Evolutionary advancement parameters of mixed pathway metabolites of *Solanum* species; codes are: AF (*African non-spiny*), A (*Archaesolanum*), L (*Leptostemonum*), B (*Brevantherum*), G (*Geminata*), C (*Cyphomandra*), D (*Dulcamaroid*), M (*Morelloid*), P (*Potato*)

Code	Species	Mixed Pathway					
		EA_G	EA_M	EA_{TP}	EA_{TU}	EA_O	EA_E
AF	*S. guineense*	0.3333	0.2222	0.5556	0.4444	0.3556	1.6889
A2	*S. laciniatum*	0.3750	0.1250	0.5000	0.5000	0.2500	0.8333
L4	*S. aethiopicum*	0.0000	0.0000	0.0000	1.0000	0.2667	0.0000
L5	*S. agrarium*	0.0000	0.2500	0.2500	0.7500	0.0667	0.0833
L7	*S. angustifolium*	0.1000	0.0000	0.1000	0.9000	0.2667	0.2222
L8	*S. anguivi*	0.1000	0.0000	0.1000	0.9000	0.2667	0.2222
L19	*S. citrullifolium*	0.0476	0.4762	0.5238	0.4762	0.0741	0.2522
L20	*S. coagulans*	0.1857	0.0643	0.2500	0.7500	0.1238	0.2630
L24	*S. elaeagnifolium*	0.1364	0.0000	0.1364	0.8636	0.1848	0.3243
L26	*S. glabratum*	0.0667	0.6111	0.6778	0.3222	-0.0952	0.2841
L28	*S. grayi*	0.1000	0.3000	0.4000	0.6000	0.0625	0.0816
L30	*S. heterodoxum*	0.0000	0.5000	0.5000	0.5000	0.0556	0.1886
L32	*S. incanum*	0.1333	0.0250	0.1583	0.8417	0.1240	0.1786
L34	*S. jabrense*	0.0000	0.4956	0.4956	0.5044	-0.0404	0.0870
L38	*S. macrocarpon*	0.2250	0.0000	0.2250	0.7750	0.2000	0.4444
L42	*S. palinacanthum*	0.2000	0.0000	0.2000	0.8000	0.2667	0.4444
L43	*S. paludosum*	0.0000	0.5083	0.5083	0.4917	-0.0758	0.1039
L44	*S. paniculatum*	0.2000	0.0000	0.2000	0.8000	0.2667	0.4444
L45	*S. paraibanum*	0.0000	0.6100	0.6100	0.3900	-0.1267	0.1702
L47	*S. quitoense*	0.1125	0.0500	0.1625	0.8375	0.1646	0.2378
L48	*S. rhytidoandrum*	0.0000	0.5639	0.5639	0.4361	-0.1278	0.1530
L50	*S. rostratum*	0.2125	0.0500	0.2625	0.7375	0.1979	0.2938
L52	*S. schimperianum*	0.1643	0.2214	0.3857	0.6143	0.0794	0.2806
L54	*S. sisymbrifolium*	0.1000	0.0000	0.1000	0.9000	0.2000	0.2222
L58	*S. tenuipes*	0.0476	0.4762	0.5238	0.4762	0.0565	0.2668
L59	*S. torvum*	0.0824	0.0235	0.1059	0.8941	0.1324	0.1140
L62	*S. viarum*	0.1667	0.0000	0.1667	0.8333	-0.1333	0.1175
L41	*S. melongena*	0.1956	0.0048	0.1921	0.7996	0.1567	0.1351
L53	*S. sessiliflorum*	0.0000	0.0000	0.0000	1.0000	-0.0667	0.0667
B2	*S. asperum*	0.3333	0.0000	0.3333	0.6667	0.0889	0.2771
B4	*S. cernuum*	0.2346	0.0000	0.2346	0.7654	0.1128	0.3897
B5	*S. erianthum*	0.1667	0.2083	0.2500	0.5000	-0.0261	0.4361

Code	Species	Mixed Pathway					
		EA_G	EA_M	EA_{TP}	EA_{TU}	EA_O	EA_E
G4	*S. campaniforme*	0.2500	0.0000	0.2500	0.7500	0.1333	0.4444
G10	*S. oblongifolium*	0.1000	0.1667	0.2667	0.7333	0.0333	0.2095
G13	*S. spirale*	0.0000	0.0000	0.0000	1.0000	0.1333	0.0000
G11	*S. pseudocapsicum*	0.2000	0.0000	0.2000	0.8000	0.2667	0.3651
C2	*S. betaceum*	0.1744	0.0281	0.2026	0.7974	0.1067	0.3148
C3	*S. corymbiflorum*	0.2000	0.0000	0.2000	0.8000	0.2667	0.4444
C4	*S. glaucophyllum*	0.1682	0.0182	0.1864	0.8136	0.2242	0.2720
D2	*S. crispum*	0.1889	0.0222	0.2111	0.7000	0.2000	0.3238
D3	*S. dulcamara*	0.1286	0.0000	0.1286	0.8714	0.1714	0.2086
D6	*S. lyratum*	0.1571	0.1250	0.2821	0.7179	0.0333	0.0796
D10	*S. valdiviense*	0.1000	0.0000	0.1000	0.9000	0.2667	0.1429
M1	*S. americanum*	0.1667	0.1667	0.3333	0.6667	0.1595	0.3255
M3	*S. chenopodioides*	0.0000	0.0000	0.0000	1.0000	0.2667	0.0000
M5	*S. nigrum*	0.0646	0.0338	0.0985	0.9015	0.1253	0.1380
M8	*S. retroflexum*	0.0000	0.0000	0.0000	1.0000	0.2667	0.0000
M10	*S. scabrum*	0.3067	0.1167	0.4233	0.5767	0.3133	0.5549
M13	*S. villosum*	0.0000	0.0000	0.0000	1.0000	0.2667	0.0000
P1	*S. acaule*	0.1000	0.0556	0.1556	0.7444	0.0889	0.2396
P3	*S. berthaultii*	0.1000	0.0556	0.1556	0.7444	0.0889	0.2396
P5	*S. cardiophyllum*	0.0000	0.0000	0.0000	1.0000	-0.1333	0.0000
P13	*S. demissum*	0.2000	0.0000	0.2000	0.8000	0.2667	0.4444
P16	*S. habrochaites*	0.0944	0.3000	0.3944	0.7167	0.3111	0.2146
P20	*S. jamesii*	0.1000	0.0000	0.1000	0.9000	0.3333	0.2222
P29	*S. muricatum*	0.0500	0.0000	0.0500	0.9500	0.1833	0.1278
P31	*S. neorickii*	0.0667	0.0000	0.0667	0.9333	0.3111	0.1481
P35	*S. pimpinellifolium*	0.0000	0.0000	0.0000	1.0000	0.2667	0.0000
P36	*S. pinnatisectum*	0.2000	0.0000	0.2000	0.8000	0.2667	0.3651
P41	*S. stoloniferum*	0.2250	0.0000	0.2250	0.7750	0.2000	0.3651
P25	*S. lycopersicum*	0.1437	0.0143	0.1579	0.8421	0.0730	0.1142
P43	*S. tuberosum*	0.2529	0.1238	0.3767	0.6233	0.1228	0.3003

Table 3. Variables contributions to factor 1 and 2 in factor analysis of *Solanum* species

Variable	Factor 1	Factor 2
AE_{OGly}	0,000874	0,910797
AE_{OMet}	-0,932375	-0,259984
AE_{TP}	-0,957091	0,232024
AE_{TU}	0,961883	-0,234008
AE_O	0,588039	0,561087
AE_E	-0,251698	0,896333

4. Conclusions

Preliminary chemosystematic analysis of *Solanum* species allowed an estimate of evolutionary features in the genus. Moreover, it evidences micromolecular similarity in genus systematic and evolutionary context, related to structural chemical variation.

Although it cannot be actually confirmed which subgenus is more primitive and which is more advanced, it is conclusive that the eight *Leptostemonum* species (L19, L26, L30, L34, L43, L45, L48, L58) have distinct features from other species belonging to this taxon, due to O-methylflavonoids. These species elaborate more specialized protection mechanisms by O-methylation, what could represent a transition group or even a more evolved one. An associated analysis with molecular phylogenetic and morphological characters could confirm this assumption indicated by the chemical data.

Finally, it is expected that in near future, chemosystematics analysis of metabolites from the acetic acid pathway, which predominates in *Solanum* metabolism,

could help to elucidate the evolutionary history still unresolved in this taxon.

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REFERENCES

[1] Frodin, D. G. 2004. History and concepts of big plant genera. Taxon, v. 53, n. 3, p. 753-776. https://doi.org/10.2307/4135449.

[2] Olmstead, R. G.; Bohs, L. 2007. A summary of molecular systematic research in Solanaceae: 1982-2006. Acta Horticulturae, p. 255-268. https://doi.org/10.17660/ActaHortic.2007.745.11.

[3] Dunal, M. F. 1813. Histoire naturelle, médicale et économique des *Solanum*. 257p.

[4] Dunal, M. F. 1852. Prodromus Systematis Naturalis Regni Vegetabilis. Candolle.

[5] D'arcy, W. G. 1972. Solanaceae Studies II: Typification of Subdivisions of *Solanum*. Annals of the Missouri Botanical Garden, v. 59, n. 2, p. 262-278. http://doi.org/10.2307/2394758.

[6] D'arcy, W. G. 1991. The Solanaceae since 1976, with review of its biogeography. In: Hawkes, J. G.; Lester, R. N.; Nee, M. Solanaceae III: Taxonomy, chemistry, evolution. Royal Botanical Garden & Linnean Society, p. 75-137.

[7] Nee, M. 1999. Synopsis of *Solanum* in the New World. In: Nee, M. et al. Solanaceae IV: advances in biology and utilization. Kew: The Royal Botanic Gardens.

[8] Hunziker, A. T. 2001 Genera *Solanacearum*: the genera of Solanaceae illustrated, arranged according to a new system. Ruggell, Liechtenstein: Gantner Verlag xvi, 500p.

[9] Bohs, L.; Olmstead, R. G. 1997. Phylogenetic relationships in *Solanum* (Solanaceae) based on ndhf sequences. Systematic Botany, v. 22, n. 1, p. 5-17. https://doi.org/10.2307/2419674.

[10] Bohs, L.; Olmstead, R. G. 1999. *Solanum* phylogeny inferred from chloroplast DNA sequence data. In: Nee, M. et al. Solanaceae IV: advances in biology and utilization. Royal Botanical Gardens, p. 97-110.

[11] Bohs, L. 2005. Major clades in *Solanum* based on ndhF sequence data. A Festschrift for William G. D'Arcy: the legacy of a taxonomist. Monographs in systematic botany from the Missouri Botanical Garden. p. 27-49.

[12] Weese, T. L.; Bohs, L. 2007. A three-gene phylogeny of the genus *Solanum* (Solanaceae). Systematic Botany, v. 32, n. 2, p. 445-463. https://doi.org/10.1600/036364407781179671.

[13] Roe, K. E. 1972. A revision of *Solanum* section *Brevantherum* (Solanaceae). Brittonia, v. 24, n. 3, p. 239-278. https://doi.org/10.2307/2805665.

[14] Agra, M. F.; Nurit-Silva, K.; Berger, L. R. 2009. Flora da Paraíba, Brasil: *Solanum* L. (Solanaceae). Acta Botanica Brasilica, v. 23, n. 3, p. 826-842. https://doi.org/10.1590/S0102-33062009000300024.

[15] Harborne J.B. 1977. Flavonoids and the evolution of the Angiosperms. Biochemical Systematics and Ecology, v. 5, p. 7-22. https://doi.org/10.1016/0305-1978(77)90013-8.

[16] Gottlieb, O. R.; Kaplan, M. A. C.; Borin, M. R. M. B. 1996. Biodiversidade: um enfoque químico-biológico. Editora da UFRJ.

[17] Soares, G. L. G.; Kaplan, M. A. C. 2001. Analysis of flavone-flavonol ratio in Dicotyledoneae. Botanical Journal of the Linnean Society, v. 135, p. 61-66. https://doi.org/10.1111/j.1095-8339.2001.tb02369.x.

[18] Gottlieb, O. R. 1982. Micromolecular evolution, systematics and ecology: an essay into a novel botanical discipline. Springer-Verlag. https://doi.org/10.1007/978-3-642-68641-2.

[19] Sporne, K. R. 1980. A re-investigation of character correlations among dicotyledons. New Phytologist, v. 85, n. 3, p. 419-449. http://dx.doi.org/10.1111/j.1469-8137.1980.tb03180.x.

[20] Bate-Smith, E. C. 1962. The phenolic constituents of plants and their taxonomic significance I. Dicotyledons. Botanical Journal of the Linnean Society, v. 58, p. 95-173. https://doi.org/10.1111/j.1095-8339.1962.tb00890.x.

[21] Soares, G.L.G. 1996. Polarizações da química flavonoídica em linhagens vegetais. Rio de Janeiro. Tese de Doutorado. NPPN. UFRJ. 133p.

[22] Ramos, C. C.; Sousa, A. L.; Almeida, C. M. S.; Oliveira, R. R. Unpublished data.