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Differential Metabolic and Biological Profiles of *Lychnophora ericoides* Mart. (Asteraceae) from Different Localities in the Brazilian "*campos rupestres*"

Leonardo Gobbo-Neto,[a] Thais Guaratini,[b] Cláudia Pessoa,[c] Manoel O. de Moraes,[c] Letícia V. Costa-Lotufo,[c] Roberto F. Vieira,[d] Pio Colepicolo[b] and Norberto P. Lopes*[,a]

[a]Departamento de Física e Química, Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, 14040-903 Ribeirão Preto-SP, Brazil

[b]Instituto de Química, Universidade de São Paulo, 05508-900 São Paulo-SP, Brazil

[c]Departamento de Fisiologia e Farmacologia, Faculdade de Medicina, Universidade Federal do Ceará, 60431-970 Fortaleza-CE, Brazil

[d]Embrapa Recursos Genéticos e Biotecnologia, Parque Estação Biológica, 70770-900 Brasília-DF, Brazil

Table S1. Identification of chromatographic peaks obtained for *Lychnophora ericoides* leaf extracts and data taken from HPLC-DAD-MS and HPLC-DAD-MS/MS analyses

Peak	t / min	Secondary metabolites	Observed MS TIC ions (*m/z*)	MS/MS (*m/z*)	UV_{max} / nm
1	3.7	5-*O*-*E*-caffeoylquinic acid	$[M + H]^+$ 355.1035$^{b.p.}$ $[M + Na]^+$ 377 $[(M+H) -QA]^+$ 163	355→163$^{b.p.}$	299, 325
2	4.7	6,8-di-*C*-β-glucopyranosylapigenin (vicenin-2)	$[M + H]^+$ 595.1655$^{b.p.}$ $[(M+H)-H_2O]^+$ 577	595→577, 559, 541, 529, 523, 511, 481, 475, 457$^{b.p.}$, 427, 409	271, 333
3	7.8	6,8-di-*C*-β-glucopyranosylchrysin	$[M + H]^+$ 579.1708$^{b.p.}$ $[(M+H) -H_2O]^+$ 561	579→561, 543, 525, 513, 507, 495, 465, 459, 441$^{b.p.}$, 411,393	272, 316
4	11.3	3,4-di-*O*-*E*-caffeoylquinic acid	$[M + H]^+$ 517.1355 $[(M+H) -H_2O]^+$ 499$^{b.p.}$ $[M + Na]^+$ 539	499→319$^{p.b.}$, 163	299, 324
5	12.1	3,5-di-*O*-*E*-caffeoylquinic acid	$[M + H]^+$ 517.1354 $[(M+H) -H_2O]^+$ 499$^{b.p.}$ $[M + Na]^+$ 539	499→319$^{p.b.}$, 163	300, 325
6	14.1	4,5-di-*O*-*E*-caffeoylquinic acid	$[M + H]^+$ 517.1357 $[(M+H) -H_2O]^+$ 499$^{b.p.}$ $[M + Na]^+$ 539	499→319$^{p.b.}$, 163	300, 326
7	15.0	caffeoylferuloylquinic acid[a]	$[M + H]^+$ 531.1510 $[(M+H) -H_2O]^+$ 513$^{b.p.}$ $[M + Na]^+$ 553	513→333, 319, 177$^{b.p.}$, 163	300, 324
8	16.3	caffeoylferuloylquinic acid[a]	$[M + H]^+$ 531.1512 $[(M+H) -H_2O]^+$ 513$^{b.p.}$ $[M + Na]^+$ 553	513→333, 319, 177$^{b.p.}$, 163	299, 324
9	18.0	caffeoylferuloylquinic acid[a]	$[M + H]^+$ 531.1508 $[(M+H) -H_2O]^+$ 513$^{b.p.}$ $[M + Na]^+$ 553	513→333, 319, 177$^{b.p.}$, 163	300, 325

*e-mail: npelopes@fcfrp.usp.br

Table S1. continuation

Peak	t / min	Secondary metabolites	Observed MS TIC ions (*m/z*)	MS/MS (*m/z*)	UV_{max} / nm
10	18.9	caffeoylferuloylquinic acid[a]	$[M + H]^+$ 531.1513 $[(M+H) -H_2O]^+$ 513[b.p.] $[M + Na]^+$ 553	513→333, 319, 177[b.p.], 163	299, 325
11	21.3	3,4,5-tri-*O*-*E*-caffeoylquinic acid	$[M + H]^+$ 679.1673 $[(M+H) -H_2O]^+$ 661 $[(M+H) -CAF-H_2O)]^+$ 499[b.p.] $[M + Na]^+$ 701	513→661, 499, 163[b.p.]	299, 326
12	22.0	15-hydroxyeremantholide C	$[M + H]^+$ 363.1449 $[(M+H)-H_2O]^+$ 345[b.p.]	363→345, 301 345→301, 283, 255[b.p.], 203	266
13	26.8	15-hydroxy-16α-(1'-methylprop-1'-*Z*-enyl)-eremantholide	$[M + H]^+$ 377.1612 $[(M+H)-H_2O]^+$ 359[b.p.]	377→359, 315 359→315, 297, 269, 241, 213, 203[b.p.], 175	267
14	27.8	centratherin	$[M + H]^+$ 375.1452 $[M + Na]^+$ 397	375→275, 257, 239, 229[b.p.], 211, 201, 183, 83	268
15	31.1	unidentified STL $C_{19}H_{24}O_6$	$[M + H]^+$ 349.1660 $[(M+H) -H_2O]^+$ 331[b.p.]	349→331, 241, 215, 189[b.p.], 161 331→241, 229, 215, 189[b.p.], 161	265
16	33.0	4,5-dihydro-15-desoxygoyazensolide	$[M + H]^+$ 347.1501 $[M + Na]^+$ 369	347→261, 243, 233, 215[b.p.], 187, 159, 69	265
17	34.2	4,5-dihydroeremantholide C	$[M + H]^+$ 349.1659 $[(M+H) -H_2O]^+$ 331[b.p.]	349→331, 189[b.p.], 161 331→285, 257, 217, 189[b.p.], 161	265
18	36.4	4,5-dihydro-16α-(1'-methylprop-1'-*Z*-enyl)- eremantholide	$[M + H]^+$ 363.1815 $[(M+H) -H_2O]^+$ 345[b.p.]	363→345, 203, 189[b.p.] 345→317, 219, 203, 189[b.p.], 161	264
19	38.2	*putative* 2',4',6'-trihydroxychalcone	$[M + H]^+$ 257.0809[b.p.]	257→239, 215, 179, 173, 153[b.p.]	343
20	38.4	4,5-dihydrolychnopholide	$[M + H]^+$ 361.1645[b.p.] $[M + Na]^+$ 383	361→261, 243, 233, 215[b.p.], 197, 187, 169, 83	264
21	39.3	*putative* 4,5-dihydro-16α-(1'-methylprop-1'-*E*-enyl)- eremantholide	$[M + H]^+$ 363.1815 $[(M+H) -H_2O]^+$ 345[b.p.]	363→345, 203, 189[b.p.] 345→317, 219, 203, 189[b.p.], 161	264
22	40.0	3-*O*-acetylpinobanksin	$[M + H]^+$ 315.0875[b.p.] $[(M+H) -C_2H_2O]^+$ 273	315→273, 255, 227[b.p.], 199, 181, 153	291, 335sh
23	41.8	16α-(1'-methylprop-1'-*Z*-enyl)-eremantholide	$[M + H]^+$ 361.1643 $[(M+H) -H_2O]^+$ 343[b.p.]	361→343, 215, 187[b.p.] 343→299, 281, 269, 243, 215, 187[b.p.], 159	267
24	43.7	$C_{19}H_{20}O_5$	$[M + H]^+$ 329.1379[b.p.] $[M + Na]^+$ 351	____	276
25	48.2	2',6'-dihydroxy-4'-methoxychalcone	$[M + H]^+$ 271.0980[b.p.] $[M + Na]^+$ 293	271→167[b.p.], 131	340
26	51.8	pinostrobin	$[M + H]^+$ 271.0977[b.p.] $[M + Na]^+$ 293	271→167[b.p.], 131	289, 330sh
27	55.1	*putative* 3-*O*-acetylalpinone	$[M + H]^+$ 329.1033[b.p.] $[M + Na]^+$ 351	329→287, 269, 241, 213[b.p.], 195, 167	286, 330sh

[a] positional isomers of caffeoylquinic acids which could not be distinguishable from each other. [b.p.] base peak (100% relative abundance). sh = shoulder; CAF = caffeoyl; QA = quinic acid.

Table S2. Sum of chromatographic peak areas at 275 nm obtained from the HPLC-DAD-MS analyses and grouped by secondary metabolite classes for each plant analised and their means calculated for each population. The letters indicate each location (A. Ibiraci; B. São José da Barra; C. São João Batista do Glória; D. Cocalzinho; E. Capitólio; F. Pirenópolis; G. Delfinópolis)

		chlorogenic acids	sesquiterpene lactones	*C*-glucosylflavones	flavonoid aglicones
A	I	10.9	6.3	3.8	3.1
	II	10.5	6.4	3.3	5.4
	III	10.8	6.5	3.5	4.1
	IV	8.3	6.6	4.4	3.4
	V	9.9	5.9	4.0	4.3
	mean ± SD	10.1 ± 1.1	6.3 ± 0.3	3.8 ± 0.4	4.0 ± 0.9
B	I	6.1	0.0	0.9	12.1
	II	8.8	0.0	0.4	11.8
	III	10.2	0.0	0.4	10.2
	IV	7.6	0.0	0.6	9.7
	V	7.6	0.0	0.4	12.6
	mean ± SD	8.1 ± 1.6	0.0 ± 0.0	0.6 ± 0.2	11.3 ± 1.3
C	I	3.6	0.0	0.3	13.9
	II	3.5	0.0	0.5	12.9
	III	2.5	0.0	0.4	11.1
	IV	5.8	0.0	0.9	13.5
	V	5.2	0.0	0.9	14.8
	mean ± SD	4.1 ± 1.3	0.0 ± 0.0	0.6 ± 0.3	13.2 ± 1.4
D	I	8.1	0.0	3.8	13.2
	II	9.0	0.0	4.6	10.4
	III	10.9	0.0	5.1	9.8
	IV	4.6	0.0	3.8	12.1
	V	4.1	0.0	4.0	10.9
	mean ± SD	7.4 ± 2.9	0.0 ± 0.0	4.2 ± 0.6	11.3 ± 1.4
E	I	12.7	0.0	0.6	4.5
	II	11.5	0.0	0.6	5.7
	III	11.5	0.0	1.1	5.6
	IV	11.2	0.0	0.6	5.4
	V	10.7	0.0	0.7	6.8
	mean ± SD	11.5 ± 0.7	0.0 ± 0.0	0.7 ± 0.2	5.6 ± 0.8
F	I	9.8	0.0	5.8	7.9
	II	10.2	0.0	6.1	7.8
	III	7.4	0.0	3.2	6.9
	IV	8.7	0.0	6.5	6.6
	V	9.5	0.0	5.5	8.7
	mean ± SD	9.1 ± 1.1	0.0 ± 0.0	5.4 ± 1.3	7.6 ± 0.9
G	I	3.3	0.0	0.5	15.4
	II	3.9	0.0	0.6	13.2
	III	1.5	0.0	0.5	11.7
	IV	2.1	0.0	0.7	12.6
	V	3.0	0.0	0.7	14.3
	mean ± SD	2.7 ± 1.0	0.0 ± 0.0	0.6 ± 0.1	13.4 ± 1.4

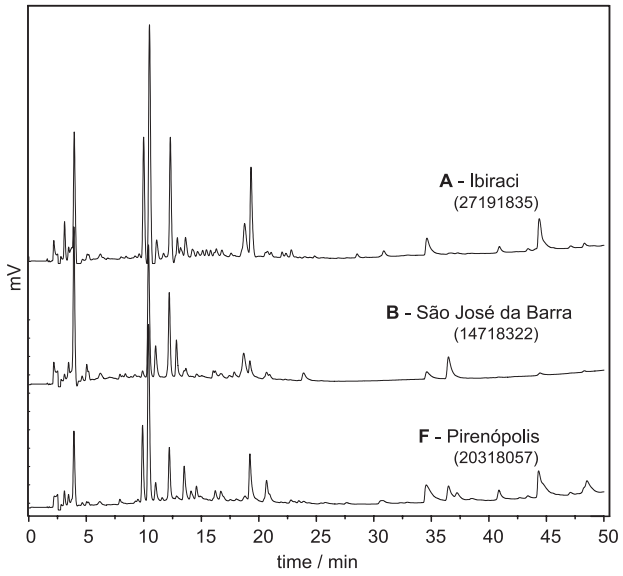

Figure S1. Representative HPLC-ECD (+500 mV) chromatograms obtained for the antioxidant leaf extracts of *Lychnophora ericoides* from the Ibiraci (A, top), Pirenópolis (F, middle) and São José da Barra (B, bottom) specimens. The number between parentheses represents the total peak area sum (chromatograms obtained at 100, 250 and 500 mV) using the same integration parameters for all the analysis.