

MATERIALS AND METHODS SUPPLEMENT 1. List of the 57 anatomical, morphological and ecological characters considered potentially useful for the phylogenetic analysis. The numbered characters correspond to those included in the analysis. The 19 characters that were excluded for at least one of the reasons detailed in the materials and methods section are marked with an asterisk.

Thallus

1. Growth form: 0 = crustose-placodioid; 1 = foliose; 2 = fruticose; 3 = squamulose.

2. Rosette presence: 0 = without well-delimited rosettes; 1 = with well-delimited rosettes; 2 = forming clusters.

Although cluster formation can be related to environmental factors, especially to the availability of organic matter, it appeared as a constant trait in the specimens of typical *C. saxicola* and sporadically in specimens of other taxa (e.g., *C. arnoldii* ssp. *obliterata*). Clauzade and Roux (1985) used this character to distinguish what they called *C. saxicola* ssp. *obliterata*, and Wetmore and Kärnefelt (1998) described one of the morphotypes of *C. saxicola* based on the formation of clusters.

3. Rosette maximum size: 0 = small (≤ 11 mm, average = 6.08); 1 = large (> 11 mm, average = 16.29).

The largest sizes were found in *C. biatorina*, *C. arnoldii* ssp. *clauzadeana* and in some specimens of *C. pusilla*.

4. Attachment to substrate: 0 = loosely attached; 1 = tightly attached.

This character was coded independently of the presence/absence of a lower cortex. The type of attachment has been often used in the literature to distinguish among different species with lobed thalli (e.g., Poelt and Hinteregger 1993, Arup 1995, Wetmore and Kärnefelt 1998). Poelt and Hinteregger (1993) differentiated *C. biatorina* based on the attachment to the substrate by means of a narrow longitudinal bundle that goes through the lobes. As we did not observe this character state it was not considered.

5. Thallus color: 0 = yellow glaucous (240); 1 = yellow (211-215, 226-230, 242-245); 2 = ochraceous-orange (246-247); 3 = orange (196-197); 4 = lead red, scarlet-orange, “terra cotta” (181-182); 5 = brownish-orange (186-187, 191-193, 201-203); 6 = salmon (169-170, 174-175, 179-180, 183-185, 189-190, 194-195, 198-200, 204-205); 7 = red (151-153, 156-158, 166-168); 8 = dark red, burgundy (171-173).

The numbers in parentheses refer to the color-coding that follows the Code Universel des Couleurs (Séguy 1936). The character states were ordered from the lightest color (yellow) to the darkest (red).

***Thallus thickness:** μm .

6. Pruina on upper cortex: 0 = absent; 1 = present.

***Upper cortex thickness:** μm .

7. Upper cortex texture: 0 = para-scleroplectenchymatous; 1 = scleroplectenchymatous type A; 2 = scleroplectenchymatous type B; 3 = sclero-prosoplectenchymatous.

Definitions following Gaya (2005, 2009).

*Upper cortex cells diameter: μm .

8. Pseudocyphella-like discolored patches presence: 0 = absent; 1 = present.

In some taxa, such as *C. rouxii*, discolored patches on the surface of the thallus are present, as a result of the irregular thinning of the upper cortex. These can resemble true pseudocyphella, and were coded as present.

*Algal layer thickness: μm .

*Algal cell diameter: μm .

*Medulla density: 0 = lax; 1 = dense.

*Hypha thickness in medulla: μm .

9. Lower cortex presence: 0 = absent; 1 = present.

The presence of a lower cortex allows the separation of the three *Xanthoria* species from *Caloplaca*.

10. Rhizine or hapter presence: 0 = absent; 1 = present.

Their presence also characterizes the three *Xanthoria* species.

11. Areole presence: 0 = absent; 1 = present.

12. Areole shape I: 0 = flat; 1 = convex.

*Areole shape II: 0 = polygonal; 1 = irregular, lobe fragments; 2 = granular or verrucose.

13. Lobe-habit I: 0 = decumbent, dorsiventral, prostrate; 1 = rising at the apex, prominent, erect.

14. Lobe-habit II: 0 = flat; 1 = convex; 2 = strongly convex, subcylindrical.

15. Lobe-habit III: 0 = not broadening at the apex; 1 = broadening at the apex.

16. Lobe-habit IV: 0 = non-contiguous, non-overlapping; 1 = contiguous, overlapping.

17. Lobe division type: 0 = simple 1 = branched/divided 2 = highly branched (2-3 times).

18. Lobe maximum length: 0 = short lobes (average = 0.92 mm); 1 = long lobes (average = 2.61 mm).

19. Lobe maximum width: 0 = narrow lobes (average = 0.54 mm); 1 = broad lobes (average = 0.92 mm); 2 = very broad lobes (average = 1.31 mm).

20. Vegetative propagule presence: 0 = absent; 1 = present.

We decided to include both soredia and isidia, without distinguishing the two, as in our study we only had three occurrences of vegetative propagules: two taxa with soredia (*C. decipiens*, *X. candelaria*) and one with isidia (*X. sorediata*).

*Pycnidium length: μm .

*Pycnidium width: μm .

Apothecium

21. Apothecium presence: 0 = absent (or rarely present); 1 = present (always present).

The presence of apothecia in *C. decipiens* has been mentioned in the literature (e.g., Poelt 1954, 1969, Wade 1965, Versegly 1970, Nordin 1972, Egea 1984, Purvis et al 1992, Wetmore and Kärnefelt 1998) always stressing its rarity. In our study, all examined specimens did not have apothecia. Therefore, we attributed state 0 to *C. decipiens*. The same state was allocated to *Xanthoria candelaria* and *X. sorediata*. The sporadic occurrence of apothecia is known from *X. candelaria* (Clauzade and Roux 1985, Poelt and Petutschnig 1992a, b, Purvis

et al 1992, Lindblom 1997) and, still more infrequently, from *X. soreliata* (Clauzade and Roux 1985, Poelt and Petutschnig 1992a, Giralt et al 1993, Lindblom 1997), but the specimens here considered were not fertile.

22. Apothecium type: 0 = pseudolecianorine; 1 = lecanorine; 2 = zeorine.

23. Apothecium location: 0 = dispersed; 1 = grouped; 2 = forming clusters.

***Apothecium diameter:** μm .

24. Pruina on apothecium: 0 = absent; 1 = present.

***Disk shape:** 0 = concave; 1 = flat; 2 = convex.

25. Disk color: 0 = yellow glaucous (240); 1 = yellow (211-215, 226-230, 242-245); 2 = ochraceous-orange (246-247); 3 = orange (196-197); 4 = lead red, scarlet-orange, "terra cotta" (181-182); 5 = brownish-orange (186-187, 191-193, 201-203); 6 = salmon (169-170, 174-175, 179-180, 183-185, 189-190, 194-195, 198-200, 204-205); 7 = red (151-153, 156-158, 166-168); 8 = dark red, burgundy (171-173).

***Margin persistence of mature apothecium:** 0 = not persistent; 1 = persistent.

26. Margin height of mature apothecium: 0 = not prominent; 1 = prominent.

27. Margin texture of mature apothecium: 0 = smooth; 1 = granulose, rugose; 2 = slightly crenulate.

28. Hymenium maximum height: 0 = short (average = 64.58 μm); 1 = tall (average = 83.71 μm).

29. Parathecium maximum thickness: 0 = narrow (average = 70.32 μm); 1 = wide (average = 102.93 μm).

***Hypothecium type:** 0 = para-scleroplectenchymatous; 1 = scleroplectenchymatous type A; 2 = scleroplectenchymatous type B; 3 = sclero-prosoplectenchymatous.

***Algal arrangement in apothecium:** 0 = more or less continuous; 1 = forming distinct clusters.

***Hyphal arrangement below the algal layer in apothecium:** 0 = lax; 1 = compact.

30. Ascus maximum length: 0 = short (average = 51.28 μm); 1 = medium (average = 60.92 μm); 2 = long (average = 66.87 μm).

31. Ascus maximum width: 0 = very narrow (average = 12.13 μm); 1 = narrow (average = 14.52 μm); 2 = broad (average = 16.38 μm); 3 = very broad (average = 18.34 μm).

32. Paraphysis branching pattern: 0 = slightly branched; 1 = highly branched (more than two divisions).

When describing species within the *C. saxicola* group (Gaya 2009), the type of branching, the degree of anastomosis, and the broadening of the apical cell were considered. However, in face of the impossibility of establishing clear limits for these characters, and given their high intraspecific variability, we thought more appropriate to code only the degree of branching, the only character that could be coded objectively.

***Paraphysis thickness at apex:** μm .

***Broadened cell number:** 0 = no cell; 1 = one cell; 2 = two or more cells (moniliform).

33. Ascospore length: 0 = short (average = 10.41 μm); 1 = long (average = 12.66 μm).

- 34. Ascospore width:** 0 = very narrow (average = 4.73 μm); 1 = narrow (average = 5.64 μm); 2 = wide (average = 6.24 μm); 3 = very wide (average = 7.24 μm).
- 35. Ascospore equatorial thickening (“septum”):** 0 = narrow (average = 2.74 μm); 1 = wide (average = 3.53 μm).
- 36. Ascospore shape (Length/Width ratio, L/W):** 0 = wide ellipsoid (average = 1.95 μm); 1 = narrow ellipsoid (average = 2.41 μm).
- 37. Ascospore length/equatorial thickening (“septum”), (L/Sept):** 0 = equatorial thickening approx. 1/3 of the spore length (average = 3.2 μm); 1 = equatorial thickening approx. 1/4 of the spore length (average = 3.83 μm); 2 = equatorial thickening approx. 1/5 of the spore length (average = 5.07 μm); 3 = equatorial thickening nearly inexistent, approx. 1/19 of the spore length, spores typically septate (average = 18.85 μm).

Ecology and Distribution

- 38. Substrate type:** 0 = carbonate rock; 1 = non-carbonate rock; 2 = igneous rock; 3 = moss.
- *Biogeographic distribution:** 0 = mediterranean/submediterranean; 1 = montane; 2 = subalpine/alpine/boreal.

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MATERIALS AND METHODS SUPPLEMENT 2.

PARAMETER DESCRIPTION FOR THE THREE SUBSTITUTION MODELS SELECTED IN THE THREE ML SEARCHES

TrN+G (Tamura and Nei 1993) in HLRT (ML1): base frequencies (A = 0.1912, C = 0.3023, G = 0.2683, T = 0.2383), rate substitution matrix (A \leftrightarrow C = 1.0000, A \leftrightarrow G = 2.8920, A \leftrightarrow T = 1.0000, C \leftrightarrow G = 1.0000, C \leftrightarrow T = 5.3436, G \leftrightarrow T = 1.0000), and rates for variable sites assuming to follow a gamma distribution with shape parameter 0.2418.

GTR+I+G (Lanave et al 1984) in AIC (ML2): base frequencies (A = 0.1791, C = 0.3093, G = 0.2787, T = 0.2328), rate substitution matrix (A \leftrightarrow C = 1.1869, A \leftrightarrow G = 3.8086, A \leftrightarrow T = 2.6292, C \leftrightarrow G = 0.8630, C \leftrightarrow T = 6.7783, G \leftrightarrow T = 1.0000), rates for variable sites assuming to follow a gamma distribution with shape parameter 0.7269, and proportion of invariable sites I = 0.4204.

HKY+G (Hasegawa-Kishino-Yano 1985) in the HLRT calculated in PAUP* with a top-down approximation (ML3): base frequencies (A = 0.1797, C = 0.3146, G = 0.2571, T = 0.2486), ti/tv ratio = 2.1501, and rates for variable sites assuming to follow a gamma distribution with shape parameter 0.2238

CONVERGENCE EXAMINATION IN BALI-PHY ANALYSES

Determining stabilization times

In order to determine the number of initial iterations to discard as burnin, we determined stabilization times for each numerical parameter and for the likelihood, prior, probability, and total tree length. We additionally computed stabilization times for the following quantities for each partition and for the total alignment: the parsimony tree length, the number of indel events, the summed length of all indel events, and the alignment length. After initially examining these values by visual inspection using the software Tracer (Rambaut and Drummond 2007), we proceeded to design a specific criterion for assessing stabilization. We counted a particular series of values as having stabilized after the series crosses its upper and then lower 90% confidence bounds twice (if the initial value is below the median) or crosses its lower and then upper confidence bounds twice (if the initial value is above the median). Here the confidence bounds are those based on its equilibrium distribution as calculated from the last third of the values in the sequence. According to this criterion, every sequence of values from each of the 6 runs in the B2 analysis stabilized by iteration 227.

We also wished to assess the stabilization of topologies, because the stabilization of log likelihood values and continuous parameter values need not imply that the topology has stabilized (Nylander et al 2008). Therefore, the Robinson-Foulds (1981) distance of the topology at each iteration from the equilibrium distribution of topologies following Redelings and Suchard (2007) were compared. We then approximated the equilibrium distribution by collecting 100 widely spaced tree samples from the last third of each of the 6 runs to obtain a total of 600 trees. Using the stabilization criterion described above, we found that this distance to the equilibrium stabilized by iteration 1320 in each of the 6 runs of the B2 analysis.

Determining Potential Scale Reduction Factors

We assessed convergence after stabilization by computing potential scale reduction factors (PSRF) based on the length of 80% credible intervals (Brooks and Gelman 1998). The PSRF is customarily considered to be small enough if it is less than 0.01. This convergence diagnostic gives a criterion for detecting when a parameter value has stabilized at different values in several independent runs, indicating a lack of convergence. This situation might occur if different runs of

the Markov chain were trapped in different modes and failed to adequately mix between modes. We computed a PSRF for every continuous model parameter, and also for the likelihood, the prior, the probability, and the total tree length. In each case the PSRF was less than 1.002, and so no lack of convergence was detected.

Effective Sample Sizes (ESS) for split frequencies

We also estimated effective sample sizes for the posterior probability of each split with $PP > 0.1$. A series of binary values for each split that indicates whether it is supported (1) or unsupported (0) in each iteration were constructed. We then computed the integrated autocorrelation time for this binary sequence in order to compute an effective sample size for each split; the larger the autocorrelation time, the smaller the effective sample size. For every split, after removing the first 10 000 values from each run as burnin and pooling the remaining values, the effective sample size for the combined result was greater than 782, and in most cases near the maximum of 54 000. This indicates that, even in the case of the worst mixing partition, we still obtained the equivalent of about 782 independent samples. While this does suggest that the estimate of the posterior probability for this split has a higher variance than other splits, an effective size of 782 indicates that none of the 6 runs had a substantially different mean.

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