BIODIVERSITAS
Volume 27, Number 3, March 2026
Pages: 15

ISSN: 1412-033X
E-ISSN: 2085-4722
https://doi.org/10.13057/biodiv/d270302

Environmental correlates of the distribution of (E,E)-farnesol-rich *Bothriochloa* species (Poaceae) in South America

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Manuscript received: 23 December 2025. Revision accepted: 3 March 2026.

Abstract. *Scrivanti LR. 2026. Environmental correlates of the distribution of (E,E)-farnesol-rich* Bothriochloa *species (Poaceae) in South America. Biodiversitas 27 (3): d270302. https://doi.org/10.13057/biodiv/d270302.* The genus *Bothriochloa* (Poaceae: Andropogoneae) comprises aromatic grasses, with several South American species reported to be rich in the oxygenated sesquiterpene (E,E)-farnesol. This compound exhibits significant pharmacological potential, including anti-obesity, antidiabetic, and anticancer activities. Despite its ecological and applied relevance, the environmental factors associated with the distribution of (E,E)-farnesol-rich *Bothriochloa* species remain poorly understood. This study evaluated the environmental correlates of the distribution patterns of ten South American *Bothriochloa* species characterized by high (E,E)-farnesol content, with the aim of identifying climatic and edaphic variables associated with their occurrence. Georeferenced occurrence records were compiled for ten *Bothriochloa* species and integrated with climatic and soil variables from the WorldClim and SoilGrids databases. Species distribution models (SDMs) were developed using Maxent to predict suitable habitats and to assess the relative contribution of environmental predictors. Model performance was evaluated using the area under the receiver operating characteristic curve (AUC), and variable importance was examined through permutation importance and jackknife tests. Most models showed high predictive performance, although some species were represented by a limited number of occurrence records, and predictions for these taxa should therefore be interpreted with caution. Climatic variables related to temperature stability, precipitation seasonality, and vapour pressure, together with edaphic factors such as soil pH and bulk density, consistently contributed to habitat suitability, although their relative importance varied among taxa. Suitable habitats were predicted across broad regions of South America, highlighting both widespread and geographically restricted distribution patterns among species. These results indicate that the distribution of (E,E)-farnesol-rich *Bothriochloa* species is associated with gradients of thermal constancy, moisture availability, and soil properties. Although the models do not directly address secondary metabolite production, they provide an ecological framework for understanding the environmental contexts in which these taxa occur, with potential implications for conservation planning, sustainable bioprospecting, and future ecological and phytochemical research on aromatic plants.

Keywords: Bioclimatic variables, edaphic variables, Maxent, sesquiterpenes, species distribution modeling

INTRODUCTION

The genus *Bothriochloa* Kuntze (Poaceae) comprises about 40 species widespread in warm-temperate and subtropical regions worldwide. In the Americas, 22 species are recognized, of which about 12 native taxa show disjunct distributions between North and South America, while three species are endemic to South America (Allred and Gould 1983). *Bothriochloa* is a well-known aromatic grass genus, particularly noted for its sesquiterpenoid compounds. Old World species are characterized by sesquiterpenes such as intermedeol, neointermedeol, and acorenone-B (Kaul and Vats 1998). In contrast, South American species exhibit a distinctive chemical profile dominated by oxygenated sesquiterpenes, including (E,E)-farnesol, γ-gurjunene, and epi-α-cadinol. Among these, (E,E)-farnesol is of particular interest as it has been reported exclusively in South American *Bothriochloa* taxa and occurs in unusually high concentrations (Scrivanti et al. 2009), suggesting a unique evolutionary and ecological specialization within the genus.

(E,E)-farnesol is an acyclic sesquiterpene alcohol with diverse biological activities and recognized pharmacological potential. Experimental studies have demonstrated its therapeutic potential against obesity, diabetes, hyperlipidemia, and atherosclerosis, as well as anticancer activity by suppressing the proliferation of a wide range of human tumor cell types—including oral squamous carcinoma, colon carcinoma, lung carcinoma, pancreatic adenocarcinoma, breast carcinoma, and leukemia—by inducing apoptosis and acting as a potent chemo-preventive agent (Lee et al. 2015). In addition, (E,E)-farnesol exhibits strong antimicrobial and antibiofilm activity, particularly against pathogenic fungi and bacteria (Alves et al. 2013; Carreiro et al. 2018; Tan et al. 2024), making it a promising bioactive molecule for pharmaceutical and biomedical applications. Although E,E)-farnesol also occurs in other plants, South American *Bothriochloa* species represent an exceptionally rich and underexplored natural source, highlighting their potential importance for pharmaceutical and biotechnological applications.

Previous studies have shown that terpenoid biosynthesis can be influenced by environmental factors such as soil properties, temperature, humidity, and altitude, particularly under warm, dry conditions associated with plant stress responses (Gershenzon 1984; Holopainen and Gershenzon 2010). Consequently, species occupying similar environmental setting may exhibit comparable chemical profiles, suggesting that environmental filtering can be associated with patterns of chemical specialization (Peñuelas and Llusià 2001; Vokou et al. 2003). TIn heterogeneous landscapes, climatic and edaphic gradients interact across spatial scales, shaping both species distributions and the environmental contexts in which chemically specialized taxa occur. Within this framework, species distribution modeling (SDM) provides a useful correlative approach to link species occurrences with environmental variables and to identify areas of suitable habitat at broad spatial scales. SDMs have been increasingly applied to aromatic and medicinal species to explore habitat suitability and environmental associations related to the occurrence of taxa characterized by specific secondary metabolites (Hosseini et al. 2024; Wani et al. 2024; Hojati et al. 2025). While SDMs do not identify direct physiological or biochemical mechanisms, they allow the characterization of environmental contexts shared by chemically defined taxa and support the generation of testable hypotheses regarding environmental filtering and niche differentiation. Despite the distinctive chemistry of South American *Bothriochloa* species, few studies have examined the environmental correlates associated with the distribution of taxa rich in (E,E)-farnesol. Understanding these associations is particularly relevant for identifying environmentally suitable areas, assessing potential vulnerability to environmental change, and informing conservation and sustainable-use strategies for chemically valuable grass species.

Here, it is hypothesized that (E,E)-farnesol-rich species of *Bothriochloa* are associated with specific environmental conditions, and that suitable distribution areas can be effectively predicted using climatic and edaphic variables. It is expected that (E,E)-farnesol-rich *Bothriochloa* species share broad classes of environmental predictors related to climatic stability (e.g., temperature variability and precipitation seasonality) and soil properties, reflecting common environmental associations across taxa characterized by this compound. At the same time, the relative importance of individual predictors is expected to vary among species, indicating heterogeneity in environmental associations within this shared framework. Differences among taxa are therefore interpreted as variation in modeled environmental suitability patterns. In this context, this study aims to identify environmentally suitable habitats for South American *Bothriochloa* species characterized by (E,E)-farnesol content, and to determine the environmental variables that most strongly influence their suitable distribution. By integrating occurrence data with climatic and soil variables within a species distribution modeling framework, this study provides insights into the environmental associations and distributional patterns of chemically characterized grasses.

MATERIALS AND METHODS

Study species and occurrence data

The oxygenated sesquiterpene (E,E)-farnesol was detected as a major component of the essential oils of 10 South American species of *Bothriochloa*: *Bothriochloa alta* (Hitchc.) Henrard, *Bothriochloa barbinodis* (Lag.) Herter, *Bothriochloa eurylemma* M. Marchi & Longhi-Wagner, *Bothriochloa imperatoides* (Hack.) Herter, *Bothriochloa laguroides* (DC.) Herter, *Bothriochloa longipaniculata* (Gould) Allred & Gould, *Bothriochloa meridionalis* M. Marchi & Longhi-Wagner, *Bothriochloa perforata* (Trin. ex E. Fourn.) Herter, *Bothriochloa saccharoides* subsp. *australis* Scrivanti, and *Bothriochloa springfieldii* (Gould) Parodi (Scrivanti et al. 2009). All 10 *Bothriochloa* species included in this study are native to South America. Accordingly, the occurrence dataset comprises only records from their native distributions, ensuring that the analyses reflect environmental associations within the species' natural range. The selection includes all *Bothriochloa* taxa known to produce (E,E)-farnesol as a primary constituent of the essential oil. Remaining species from the region were excluded due to the absence or low concentrations of this compound in their reported chemical profiles. In these species, E,E-farnesol concentrations ranged from 11.9% to 74% in their essential oils (Scrivanti et al. 2009). The chemical compositions of the species treated here are reported in Scrivanti et al. (2009).

Occurrence records for the 10 species were obtained from field collections, published studies, herbarium specimens (AAU, ASU, AU, B, CEN, CGMS, COL, CORD, CPAP, ECT, F, FLOR, FMB, G, HDCF, HVAT, ICN, LUSC, MO, MPUC, NY, S, SI, SP, SPF, U, US) and the Global Biodiversity Information Facility (http://www.gbif.org/). Records before 1950 were not used in model fit because the current climate layers cover from 1950 to 2000 (Fick and Hijmans 2017). When occurrence records lacked exact geographic coordinates, localities were georeferenced in Google Earth using the original label information. Records with vague or ambiguous locality descriptions that did not allow confident georeferencing were excluded from the dataset. For georeferenced records, an uncertainty threshold of approximately 1 km was assumed, consistent with the spatial thinning distance applied before model calibration. The locations of each specimen were transformed into geographic coordinates using a WGS84 datum that was visualized in QGIS 3.34.9. The number of occurrence records reported for each species corresponds to the final dataset used for modelling, after spatial thinning: 53 for *B. alta*, 97 for *B. barbinodis*, 9 for *B. eurylemma*, 19 for *B. imperatoides*, 25 for *B. longipaniculata*, 240 for *B. laguroides*, 11 for *B. meridionalis*, 25 for *B. perforata*, 247 for *B. saccharoides* subsp. *australis*, and 66 for *B. springfieldii* in South America.

A list of voucher specimens and examined material is provided includes detailed information on the number of records removed during each filtering step for each taxon (Table 1). Spatial thinning was applied using a minimum distance of 1 km to reduce spatial clustering and sampling bias in occurrence records. Although environmental predictors were represented at a coarser resolution (~5 km), a finer thinning distance was deliberately chosen to avoid excessive data loss and to retain sufficient occurrences, particularly for species with low sample sizes. Previous studies have shown that thinning distances smaller than the environmental resolution can effectively mitigate sampling bias while preserving biologically meaningful information (Boria et al. 2014; Fourcade et al. 2014). Thinning was implemented using the spThin package in R (Aiello-Lammens et al. 2015), after duplicate removal and coordinate uncertainty filtering, retaining a single occurrence within each 1 km radius. This approach reduces artificial spatial clustering -a common issue in presence-only modeling- and is widely recommended when integrating heterogeneous data sources or handling limited sample sizes. While additional bias correction methods exist (e.g., bias files), spatial thinning was considered the most appropriate and conservative strategy given the comparative and exploratory objectives of this study. For subsequent species distribution modelling (SDM), these occurrence datasets were partitioned using the subsample method, randomly assigning 75% of records to training and 25% to testing in each replicate run.

Environmental data and variable selection

All environmental layers used in the analyses were obtained from publicly available global datasets. Climatic data were obtained from the WorldClim database version 2.0 (Fick and Hijmans 2017), which provides 19 bioclimatic variables (Bio1-Bio19) summarizing temperature and precipitation patterns at a spatial resolution of 2.5 arc-minutes (~5 km). In addition to these bioclimatic variables, two climatic variables available in WorldClim -solar radiation, and vapor pressure- were also considered because of their ecological relevance for plant physiological performance.

Five edaphic variables were extracted from the SoilGrids database (http://soilgrids.org/) at a spatial resolution of 0.5-arc-minute (~ 1 km). These included bulk density (BDOD), soil pH (pH), soil organic carbon (SOC), and soil texture fractions of sand and silt (SAND, SILT), all extracted at a soil depth of 0-5 cm. This depth represents the topsoil horizon most directly associated with nutrient cycling and plant-environment interactions in grassland ecosystems (Weil and Brady 2016). Deeper soil layers were not included to avoid increasing model complexity without improving ecological interpretability at the continental scale. Consequently, edaphic predictors are interpreted as representing regional soil gradients rather than local soil conditions. All environmental rasters were aligned to a common spatial grid prior to model calibration. Climatic layers from WorldClim (2.5 arc-minutes resolution) were used as the reference grid to ensure consistency with the spatial resolution commonly applied in continental-scale species distribution modelling. Edaphic variables from SoilGrids (0.5 arc-minutes resolution) were resampled to match the spatial resolution (2.5 arc-minutes), projection (WGS84; EPSG:4326), geographic extent, and grid alignment of the WorldClim reference raster using the GDAL "Warp (reproject)" algorithm implemented in QGIS v3.34.9. Because soil predictors represent continuous variables, resampling from 1 km to 5 km resolution was performed using bilinear interpolation, which computes a distance-weighted average of neighbouring cells and is appropriate for continuous environmental surfaces (Hijmans et al. 2005; Franklin 2010). All layers were clipped to a common South American extent, and binary consensus mask was generated by identifying the spatial intersection of valid pixels across all predictor variables.

Given the limited number of species occurrences, the retention of presence was prioritized to maximize statistical power. For occurrence points falling on NoData cells a localized gap-filling procedure was applied using nearest-neighbor interpolation in QGIS to assign the value of the closest valid pixel. This ensured a continuous and consistent environmental surface across all predictors, preventing the exclusion of occurrence points during model calibration and background sampling in MaxEnt (Phillips et al. 2006). Together with the prior raster alignment and resampling procedures, this harmonization procedure ensured that all environmental variables contributed to the models on a comparable spatial basis, avoiding biases associated with mixed spatial resolutions (Elith and Leathwick 2009; Franklin 2010).

To reduce multicollinearity among environmental predictors, pairwise Pearson correlation coefficients were calculated across all terrestrial pixels within the harmonized South America extent after raster alignment and masking. Correlations were computed using the full set of spatially overlapping grid cells shared by all predictors. When two variables were highly correlated ($r \geq 0.80$), one variable from each correlated pair was excluded. The selection of the retained variable within each correlated pair was based on its biological relevance for the group, supported by previous ecological and biogeographical studies conducted on *Bothriochloa* and other grass genera from South America (Quiroga et al. 2018; Zielińska et al. 2024; Scrivanti and Anton 2025). As a result, several temperature- and precipitation-related bioclimatic variables showing strong collinearity with the retained predictors (Bio4, Bio5, Bio7, Bio9, Bio10, Bio11, Bio14, Bio16, Bio17, Bio19) were excluded from model calibration. The final set of climatic predictors retained for model calibration included annual mean temperature (Bio1), mean diurnal temperature range (Bio2), isothermality (Bio3), minimum temperature of the coldest month (Bio6), mean temperature of the wettest quarter (Bio8), annual precipitation (Bio12), precipitation of the wettest month (Bio13), precipitation seasonality (Bio15), precipitation of the warmest quarter (Bio18), solar radiation (SR), and water vapour pressure (WVP). Edaphic predictors retained in the final models included BDOD, pH, SOC, SAND, and SILT. The retained predictors represent climatic and edaphic conditions known to influence water availability, thermal regimes, plant physiological stress, and the production and variability of terpenoid compounds in grassland species (Lima et al. 2003).

Table 1. Summary of occurrence data filtering and final records retained for (E,E)-farnesol-rich *Bothriochloa* species distribution modeling

Species	Initial records (South America)	Removed pre-1950	Removed due to vague locality / ID	Final records retained for modeling
Bothriochloa alta	167	89	25	53
Bothriochloa barbinodis	436	269	70	97
Bothriochloa eurylemma	33	21	3	9
Bothriochloa imperatoides	75	41	15	19
Bothriochloa laguroides	974	478	256	240
Bothriochloa longipaniculata	82	46	11	25
Bothriochloa meridionalis	22	3	8	11
Bothriochloa perforata	57	17	15	25
Bothriochloa saccharoides subsp. *australis*	927	410	270	247
Bothriochloa springfieldii	214	88	60	66

Species distribution modeling

Species distribution models (SDMs) were generated using Maxent v3.4.4 (Phillips et al. 2006), which estimates relative habitat suitability from presence-only records and environmental predictors. All models were calibrated using the harmonized environmental raster stack at 2.5 arc-minute (~5 km) resolution. Background points were sampled across South America, within the environmental extent defined by the harmonized raster stack, which established the geographic space for model calibration. This geographic domain was considered an approximation of the accessible area (Soberón and Peterson 2005) for the studied taxa.

Most *Bothriochloa* species included in this study have broad geographic distributions across South American grassland systems, including the Pampas, Chaco, Cerrado, and other open vegetation formations, suggesting long-term capacity for dispersal across these environments. Given these distributional patterns and the comparative objective of this study across ten species sharing similar ecological affinities, continent-wide background extent was considered an ecologically reasonable approximation of the accessible environmental space. The use of a shared background also avoids biases introduced by species-specific background definitions in comparative SDM frameworks (Barve et al. 2011) and follows previous biogeographical and ecological niche modeling studies on *Bothriochloa* in South America (Quiroga et al. 2018; Zielińska et al. 2024; Scrivanti and Anton 2025). However, given the wide distributions of several species and the exploratory and the comparative nature of this study, a continent-wide background was considered ecologically appropriate and methodologically consistent across species. To evaluate the robustness of model predictions, a sensitivity analysis was conducted for species with low numbers of occurrences by testing alternative background extents and regularization multipliers. The resulting models were compared with the main models in terms of spatial suitability patterns and relative importance of environmental predictors.

Models were run using default feature settings, with a regularization multiplier of 1, a maximum of 10,000 background points, 500 maximum iterations, and a convergence threshold of 0.00001. Duplicate presence records were removed automatically by the software. For each species, 100 replicate model runs were performed using the subsample method (75% training, 25% testing). This partitioning scheme and the general model configuration follow previous species distribution modeling studies conducted on *Bothriochloa* and other grass taxa with comparable occurrence dataset sizes, ensuring methodological consistency with earlier ecological niche modeling approaches applied to this group (Scrivanti and Anton 2025). Default feature classes were used for all species to ensure methodological consistency and comparability among models. Although tuning feature classes and regularization parameters can improve predictive performance for individual species, especially when optimizing single-species models, the use of uniform settings is recommended in comparative and multi-species frameworks to avoid confounding biological differences with methodological variation.

Moreover, several studies have shown that Maxent can produce reliable predictions even with relatively small sample sizes when appropriate precautions are taken to limit model complexity (Pearson et al. 2007; Wisz et al. 2008). In addition, several species included in this study had limited numbers of occurrence records, for which more complex model tuning may increase the risk of overfitting. For taxa with low sample sizes (e.g., $n \leq 11$), model complexity was indirectly controlled through prior steps including correlation filtering of predictors, spatial thinning of occurrences, and the use of a moderate number of environmental variables. These measures reduce the effective dimensionality of the models and are widely recommended when working with small presence datasets in SDM analyses (Wisz et al. 2008; Franklin 2010). Therefore, default settings were considered appropriate for the exploratory and comparative aims of this study, following common practice in large-scale ecological niche modeling studies of grasses and other plant taxa.

Model performance was evaluated using the area under the curve (AUC) of the receiver operating characteristic (ROC) plot for the test data (Fielding and Bell 1997; Phillips et al. 2006). In addition to AUC, model performance was evaluated through threshold-dependent omission rates calculated using the 10th percentile training presence threshold, a commonly applied criterion in presence-only species distribution models. This threshold allows a small proportion of training occurrences (10%) to fall below the predicted suitability threshold, accounting for potential spatial uncertainty and environmental variability in occurrence data. Test omission rates were calculated across the 100 replicate runs for each species and are reported as mean ± standard deviation. These values were used to evaluate the degree to which independent test records were correctly predicted by the models. Under the 10th percentile threshold, omission values close to the expected rate (~0.10) indicate appropriate model generalization and limited overfitting. Although AUC has known limitations, including dependence on geographic extent and prevalence, and its inability to distinguish between omission and commission errors (Lobo et al. 2008; Jiménez-Valverde 2012), it was used here as a complementary metric due to its widespread application in SDM studies, facilitating comparison with previously published results. In this context, AUC values closer to 1 indicate a higher ability of the model to discriminate between suitable and unsuitable areas. The relative importance of environmental variables was assessed using permutation importance and jackknife tests implemented within the Maxent framework. Habitat suitability maps were generated using logistic output, and binary presence-absence maps were derived using the 10th-percentile training presence threshold (Abba et al. 2012).

Pixels with values above this threshold were classified as suitable habitat, whereas values below the threshold were considered unsuitable (Phillips et al. 2006). To mitigate the risk of overfitting and enhance model robustness across species with contrasting sample sizes, several precautionary steps were implemented. Multicollinearity among predictors had been previously reduced through correlation filtering, thereby limiting model complexity while retaining ecologically interpretable variables. Occurrence records were spatially thinned to reduce the influence of clustered sampling and spatial autocorrelation. In addition, a uniform modeling strategy (default feature classes and regularization settings) was applied across all species to avoid species-specific parameter tuning that could inflate performance metrics and hinder comparability in a multi-species framework. For species with few occurrences (*B. eurylemma*, *B. imperatoides*, *B. meridionalis*), these conservative modeling choices were complemented by a deliberately cautious interpretation of model outputs, which are treated as exploratory representations of broad-scale environmental associations rather than as optimized predictive models.

RESULTS AND DISCUSSION

The Maxent models showed good discriminatory performance for the ten (E,E)-farnesol-rich *Bothriochloa* species, with AUC values ranging from 0.923 to 0.990 (Table 2). Using the 10th percentile training presence threshold, mean test omission rates ranged from 0.105 to 0.147, with an overall mean close to the expected value (~0.10) under the 10th percentile training presence threshold. These results indicate that the models showed good generalization capacity and limited overfitting. For species with relatively low numbers of occurrence records (*B. eurylemma*, *B. imperatoides*, and *B. meridionalis*), an additional sensitivity analysis was conducted by increasing the regularization multiplier (RM = 2). The resulting models showed only minor differences in AUC values and omission rates, and the same environmental predictors remained among the most influential variables (Table 3). Because percent contribution and permutation importance reflect different aspects of model behaviour in Maxent, both metrics were examined to better interpret predictor influence. Percent contribution represents the relative increase in model gain during the training process and therefore reflects how strongly a variable was used during model fitting. In contrast, permutation importance measures the decrease in model performance after randomly permuting the values of a predictor and therefore reflects the variable's independent contribution to model discrimination. Discrepancies between both metrics may arise when predictors are partially correlated or when interactions among variables occur. The jackknife test of regularized training gain indicated that climatic variables related to thermal stability and atmospheric humidity (Bio3, Bio15, WVP) were frequently ranked among the most influential predictors across species. Among edaphic variables, soil pH also showed notable importance in several models, indicating that both climatic and soil-related factors are statistically associated with patterns of habitat suitability (Table 4).

Isothermality (Bio3) showed a high percent contribution and, in several cases, high permutation importance in the SDMs of *B. eurylemma*, *B. imperatoides*, *B. longipaniculata*, *B. meridionalis*, *B. laguroides*, and *B. saccharoides* subsp. *australis*, indicating that the occurrence of these species is associated with environments characterized by relatively stable temperature regimes. In contrast, vapour pressure (WVP) showed higher importance values in the SDMs of *B. barbinodis*, *B. laguroides*, *B. springfieldii*, and *B. saccharoides* subsp. *australis,* suggesting a stronger association with atmospheric moisture conditions. Precipitation seasonality (Bio15) was also among the most influential climatic predictors for *B. imperatoides B. laguroides*, *B. alta*, *B. meridionalis*, and *B. perforata,* highlighting the relevance of seasonal rainfall regimes for these taxa (Table 4).

Table 2. Test AUC and test omission rates (10th percentile threshold) for the Maxent models of ten (E,E)-farnesol-rich *Bothriochloa* species (mean ± SD across 100 replicates)

Species	**Test AUC**	**Test omission (10% threshold)**
B. alta	0.989±0.006	0.147±0.042
B. barbinodis	0.923±0.094	0.127±0.079
B. eurylemma	0.960±0.033	0.105±0.083
B. imperatoides	0.988±0.006	0.140±0.043
B. laguroides	0.936±0.015	0.131±0.050
B. longipaniculata	0.978±0.010	0.142±0.081
B. meridionalis	0.990±0.015	0.113±0.074
B. perforata	0.968±0.031	0.115±0.079
B. saccharoides subsp. *australis*	0.943±0.012	0.109±0.054
B. springfieldii	0.961±0.019	0.139±0.071

Table 4. Percent contribution and permutation importance of environmental variables used to predict the habitat suitability of (E,E)-farnesol-rich *Bothriochloa* species. Values represent the average from 100 replicates of Maxent runs. Highly correlated variables were excluded. Bold values indicate the highest values per species

Variable	**BALTA**		**BBARB**		**BEURY**		**BIMPE**		**BLAGU**		**BLONG**		**BMERI**		**BPERF**		**BSACC**		**BSPRIN**	
	Con (%)	**Per (%)**	**Con (%)**	**Per (%)**	**Con (%)**	**Per (%)**	**Con (%)**	**Per (%)**	**Con (%)**	**Per (%)**	**Con (%)**	**Per (%)**	**Con (%)**	**Per (%)**	**Con (%)**	**Per (%)**	**Con (%)**	**Per (%)**	**Con (%)**	**Per (%)**
*AUC	0.989±0.006		0.923±0.094		0.960±0.033		0.988±0.006		0.936±0.015		0.978±0.010		0.990±0.015		0.968±0.031		0.943±0.012		0.961±0.019	
BIO1	2.7	0	16.2	44	0	0	0	0	2.5	4.2	1.1	13.2	0	0.1	3.3	0	13.6	31.3	5.7	26.4
BIO2	1.3	2.2	1	1.4	0	0.5	0.6	0	1	4	1.9	0.9	0.1	0	0.4	0.4	1	3.2	0.3	0.3
BIO3	3.4	0.3	4.7	3.9	38.4	64.3	36.4	82.2	14	10.3	39.2	60.1	35	57.8	4.1	0.1	16.2	8	0.6	1.3
BIO6	36.4	79.7	0.4	5.5	0	0.2	6.2	0.2	0.8	11.7	0.3	2.8	0	0	27.8	70.4	1.7	4.8	8.4	0.6
BIO8	0.8	0.1	3.4	2.9	3.1	0	0.1	0.1	1	2.6	0.1	0.2	0.3	0.1	5.5	0.6	5.8	5.4	10.1	10.3
BIO12	1.4	6.3	0.5	3.6	0.1	0.1	0.1	0.4	1.5	10.3	11.4	3.3	0.8	4.2	0.1	0	0.5	8.4	8.4	36.1
BIO13	0.3	0.1	0.1	0.4	0.1	0.1	0	0	0.8	4.6	2.7	4.0	0	0	2.4	4.7	5.2	1.3	0	0.1
BIO15	15.6	3.2	7.9	3.1	5.9	0.1	22.8	6.5	18.7	8.7	2.9	4.0	27.6	0.3	17.8	9.3	1.4	5.2	7.3	2.9
BIO18	2.8	0.7	6.2	0.9	2.9	4.2	0	0	11.8	2.2	15.4	0.8	2	0.8	9.7	3.8	0.1	0.3	0.7	0.2
BDOD	0.1	0	5.6	1.8	43.4	26	24.7	0.6	0.6	0.4	0.6	0.6	10.8	0	1.7	2.4	8.5	3.2	1.5	0.2
pH	1.1	0.2	13.6	26.1	1.1	0.5	1.8	1.1	2.1	24.3	0.2	0.1	15	20.8	1.4	0.9	4.6	6.3	15.5	0.4
SAND	0.5	1.4	0.2	0.7	0.1	0.3	3.8	0.5	2.6	2.1	0.9	0.1	0	0	0	0	0.6	1.6	0.7	0.6
SILT	27.4	1	3.5	1.2	3.1	0.7	0.2	0	0.9	1.4	2.7	0.6	1.1	0.1	6.9	0.9	10.3	13	8.2	4.2
SOC	4.5	4	0.1	0.6	0.8	2.4	0	0	0.7	5.5	1.5	0.2	3.2	4.9	1.7	4.2	1.3	4.5	1.4	1.3
SR	0.4	0.9	0.4	1.9	1	0.6	3.2	7.9	7.1	4	4.5	3.7	3.4	5.8	1	2.2	0.4	0.6	0.8	1
WVP	1.5	0	36.2	2.1	0	0	0.1	0.5	33.8	3.3	14.6	5.5	0.8	5.2	16.2	0.1	28.8	2.9	30.4	14

Note: BALTA: *Bothriochloa alta*, BBARB: *Bothriochloa barbinodis*, BEURY: *Bothriochloa eurylemma*, BIMPE: *Bothriochloa imperatoides*, BLAGU: *Bothriochloa laguroides*, BLONG: *Bothriochloa longipaniculata*, BMERI: *Bothriochloa meridionalis*, BPERF: *Bothriochloa perforata*, BSACC: *Bothriochloa saccharoides* subsp. *australis*, BSPRIN: *Bothriochloa springfieldii*. Con (%): percent contribution, Per (%): permutation importance. Bio1: Annual mean temperature (°C), Bio2: Mean diurnal range (mean of monthly (max temp - min temp)) (°C), Bio3: Isothermality (Bio2/Bio7) (×100), Bio6: Min temperature of coldest month, Bio8: Mean temperature of wettest quarter, Bio12: Annual precipitation (mm), Bio13: Precipitation of wettest month (mm), Bio15: Precipitation Seasonality (CV), Bio18: Precipitation of warmest quarter (mm), BDOD: Bulk density (kg/cubic-meter), pH: Soil pH, SAND: Soil texture fraction sand (%), SILT: Soil texture fraction silt (%), SOC: Soil organic carbon stock (tonnes per ha), SR: Solar radiation, WVP: Water vapour pressure. *AUC values correspond to test data and are shown for reference

Table 3. Sensitivity analysis of Maxent models for species with low numbers of occurrence records. Models were recalibrated using an increased regularization multiplier (RM = 2). Model performance metrics and the ranking of the most influential environmental predictors remained broadly consistent between model settings

Species	Regularization multiplier	Test AUC	Test omission	Top predictors
B. eurylemma	RM = 1 (default)	0.960±0.033	0.105±0.083	BDOD, Bio3
	RM = 2	0.962±0.030	0.105±0.102	Bio3, BDOD
B. imperatoides	RM = 1 (default)	0.988±0.006	0.140±0.043	Bio3, BDOD, Bio15
	RM = 2	0.989±0.005	0.189±0.124	Bio3, BDOD, Bio15
B. meridionalis	RM = 1 (default)	0.990±0.015	0.113±0.074	Bio3, Bio15, pH
	RM = 2	0.993±0.010	0.105±0.123	Bio3, Bio15, pH

Among edaphic variables, bulk density (BDOD) showed relatively high percent contribution and moderate permutation importance in the SDM of *B. eurylemma*, in combination with climatic predictors such as isothermality (Bio3). Soil pH showed higher importance values in the SDMs of *B. barbinodis*, *B. meridionalis*, and *B. springfieldii*, indicating a consistent association between species occurrence and soil chemical conditions (Table 4).

Notably, contrasts between percent contribution and permutation importance were widespread across species, although their magnitude and direction varied among predictors. In several models, variables with high percent contribution exhibited comparatively low permutation importance, including precipitation seasonality (Bio15), vapour pressure (WVP), soil texture (SILT), and bulk density (BDOD) in *B. alta*, *B. barbinodis*, *B. imperatoides*, *B. laguroide*s, *B. longipaniculata*, *B. meridionalis*, *B. perforata*, *B. saccharoides* subsp. *Australis,* and *B. springfieldii* (Table 4). This pattern indicates that these predictors contributed strongly during model fitting but shared explanatory information with other climatic or edaphic variables describing related environmental gradients, consistent with partial functional redundancy among predictors retained after correlation filtering (Table 4).

In contrast, a smaller subset of predictors exhibited both relatively high percent contribution and high permutation importance, suggesting a stronger independent role in model discrimination. Isothermality (Bio3) showed this pattern in *B. eurylemma*, *B. imperatoides*, *B. laguroides*, *B. longipaniculata,* and *B. meridionalis*, while the minimum temperature of the coldest month (Bio6) was particularly influential in *B. alta* and *B. perforata*. Additional predictors with moderate or lower percent contribution but comparatively high permutation importance included annual mean temperature (Bio1) in *B. barbinodis* and *B. saccharoide*s subsp. *australis*, as well as annual precipitation (Bio12) in *B. springfieldii*. Together, these results highlight pronounced interspecific differences in how climatic and edaphic variables contribute and structure the SDMs, while emphasizing that most predictors act as broad-scale environmental correlates rather than strict ecological thresholds (Table 4).

Response curves of the main environmental predictors (Figure 1) further illustrated the direction and shape of these associations. In several species, isothermality (Bio3) exhibited a unimodal response, with higher habitat suitability at intermediate values (approximately 45-60) and declining suitability toward lower and higher extremes, particularly in *B. eurylemma*, *B. imperatoides*, *B. laguroides*, *B. longipaniculata*, *B. meridionalis*, and *B. saccharoides* subsp. *australis*. Precipitation seasonality (Bio15) generally showed decreasing or unimodal responses, with higher suitability mostly occurring under moderate seasonal values (approximately 40-80%). Vapour pressure (WVP) displayed species-specific patterns, with higher suitability generally occurring at intermediate to moderately high values (approximately 1.21.8 kPa) in *B. barbinodis*, *B. laguroides*, *B. springfieldii*, and *B. saccharoides* subsp. *australis*, whereas in *B. perforata* its response was comparatively weak, in line with its low permutation importance. Soil pH showed unimodal responses in species such as *B. barbinodis* and *B. meridionalis*, while annual mean temperature (Bio1), which showed high permutation importance in *B. saccharoides* subsp. *australis* and *B. springfieldii*, were associated with broad suitability optima rather than sharp thresholds. Overall, the response curves support that SDM outputs reflect broad-scale, correlative environmental associations structured along gradients of temperature stability, moisture availability, and soil chemical properties.

Spatial projections of habitat suitability further revealed distinct geographic patterns across South America. Highly suitable areas for *B. alta* were concentrated in central Argentina, whereas *B. barbinodis* exhibited a broader potential range extending across central, northwestern, and northeastern Argentina, as well as southwestern and western Bolivia, western Peru, Ecuador, Colombia, and Venezuela (Figures 2.A and 2B).

Suitable habitats for *B. eurylemma* were mainly restricted to northeastern Argentina (Mesopotamia), western Uruguay, and southwestern Brazil (Figure 2.C). *B. imperatoides* showed its highest suitability in northeastern Argentina and in southern and western Uruguay (Figure 2.D). For *B. laguroides*, areas of high suitability were identified in Rio Grande do Sul (southern Brazil), Uruguay, and central, northeastern, and northwestern Argentina (Figure 2.E). *B. meridionalis* was mainly associated with northeastern Argentina, southwestern Brazil, and northern Uruguay, whereas *B. longipaniculata* showed suitable areas in northeastern Argentina, southeastern Paraguay, southwestern Brazil, and northwestern Uruguay (Figures 2.F and 2.G). Highly suitable habitats for *B. perforata* were located in central Argentina, while those of *B. saccharoides* subsp. *australis* extended broadly across central and northwestern Argentina, southwestern Bolivia, western Peru, Ecuador, Colombia, Venezuela, southwestern Brazil, and northwestern Uruguay (Figures 2.H and 2.I). Finally, *B. springfieldii* exhibited areas of high suitability mainly in central and northwestern Argentina (Figure 2.J). In most species, areas of high predicted suitability largely coincided with known occurrence records; however, in some cases, such as *B. eurylemma* and *B. saccharoides* subsp. *australis*, the models predicted suitable areas beyond currently documented occurrences (Table 5).

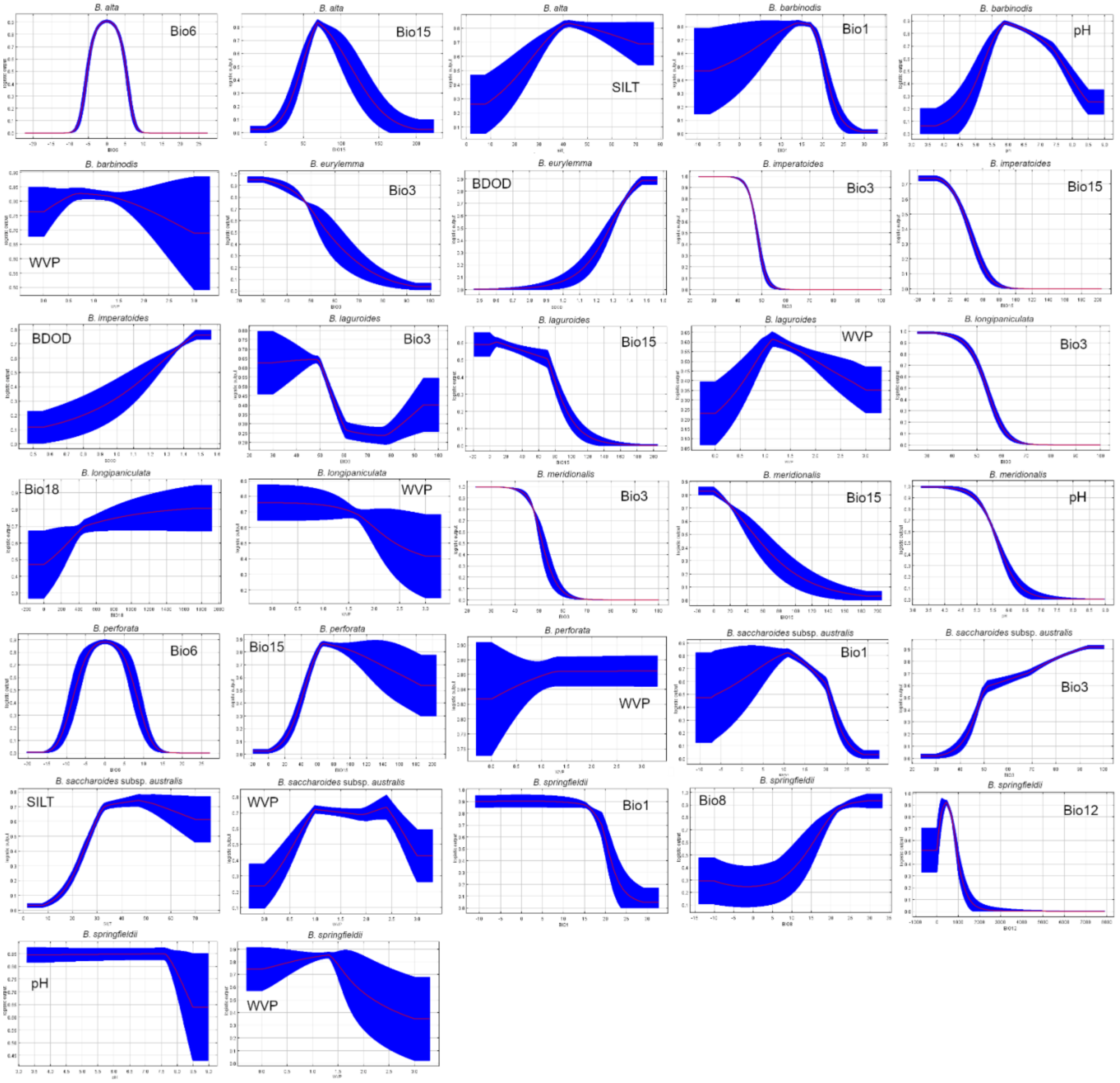
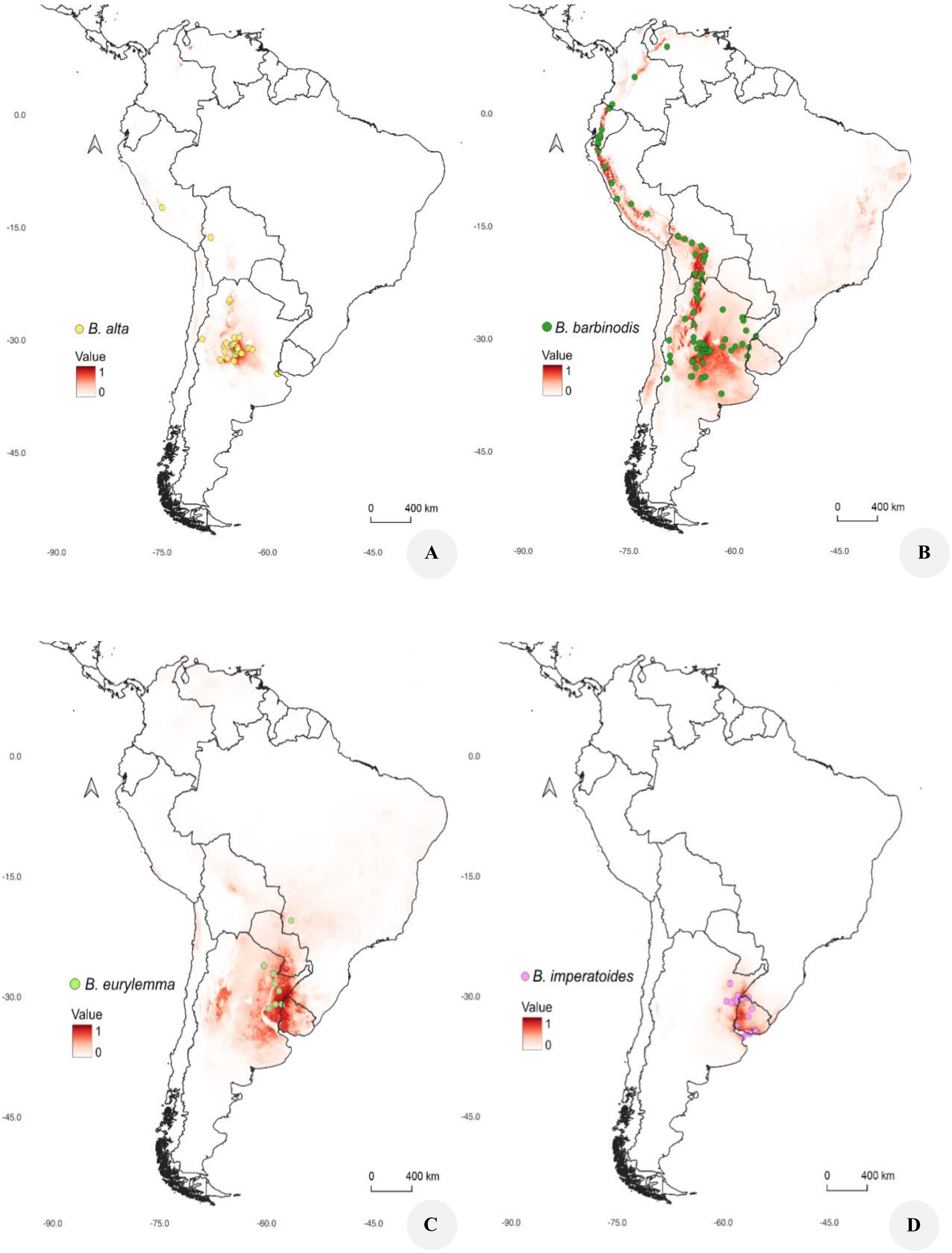
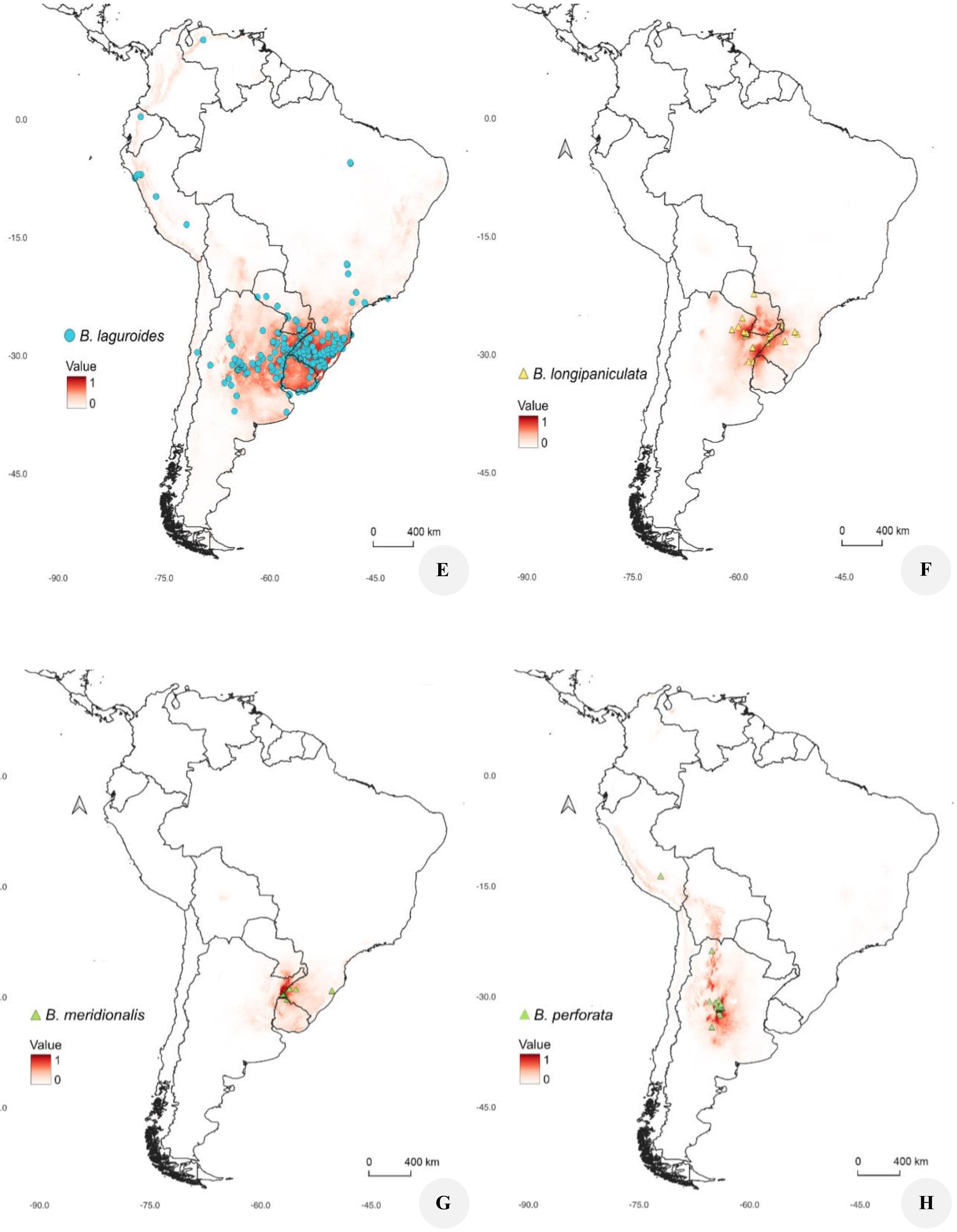


Figure 1. Response curves of the main climatic and edaphic predictors for Maxent models of (E,E)-farnesol-rich *Bothriochloa* species


B. alta
Value
1
0
0 400 km
0.0
-15.0
-30.0
-45.0
-90.0
-75.0
-60.0
-45.0
A
B. barbinodis
B
B. eurylemma
C
B. imperatoides
D


B. laguroides
Value
1
0
0.0
-15.0
-30.0
-45.0
-90.0
-75.0
-60.0
-45.0
0
400 km
E
B. longipaniculata
Value
1
0
F
B. meridionalis
Value
1
0
G
B. perforata
Value
1
0
H

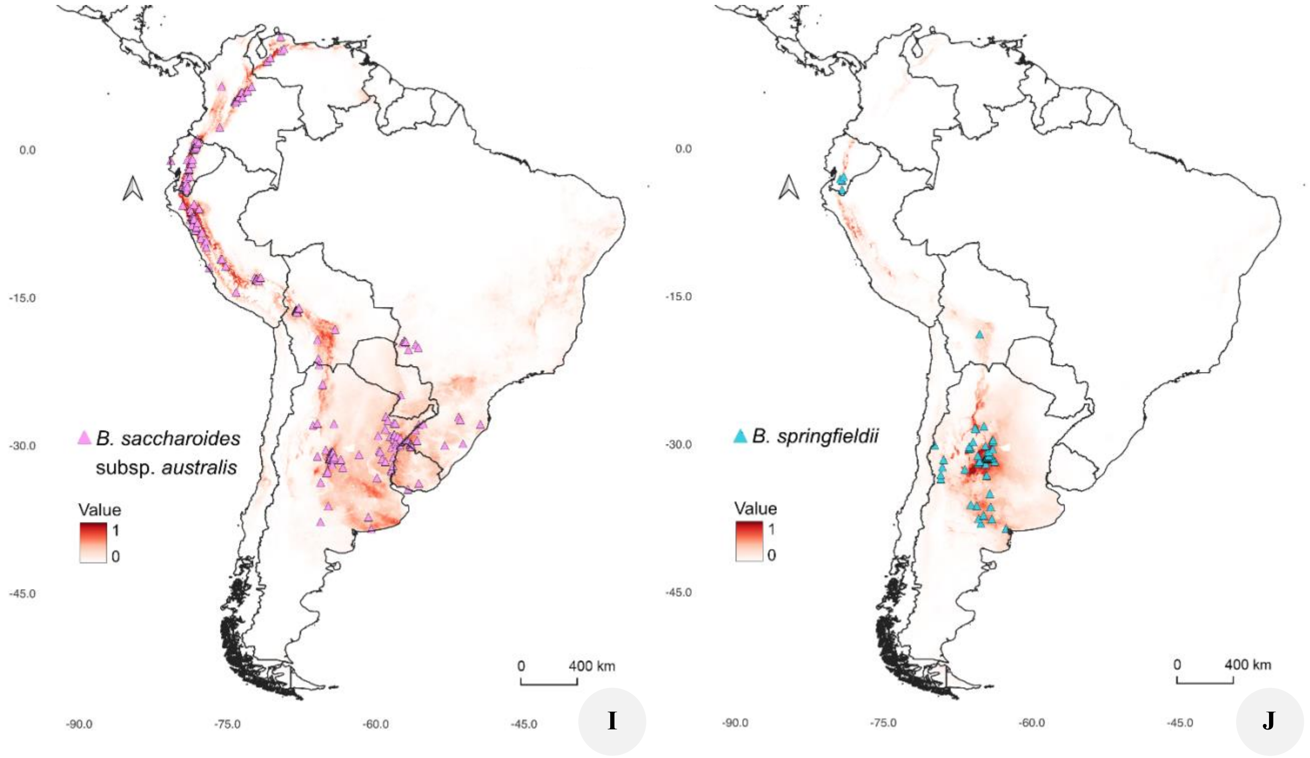


Figure 2. Niche suitability modeled with Maxent for each *Bothriochloa* species studied in South America. E: *Bothriochloa laguroides*, F: *Bothriochloa longipaniculata*, G: *Bothriochloa meridionalis*, H: *Bothriochloa perforata*, I: *Bothriochloa saccharoides* subsp. australis, J: *Bothriochloa springfieldii*. The color gradient from white to red represents increasing niche suitability. The values for habitat suitability ranged between 0 (unsuitable) and 1 (highly suitable). Suitable areas were identified using the 10th percentile training presence thresholds, corresponding to occurrence probability values of 0.2238 (*B. laguroides*), 0.3316 (*B. longipaniculata*), 0.3637 (*B. meridionalis*), 0.2744 (*B. perforata*), 0.1714 (*B. saccharoides* subsp. *australis*), and 0.3196 (*B. springfieldii*) representing the minimum predicted suitability considered climatically suitable

Table 5. Core regions of predicted habitat suitability and correspondence with known distributions for the ten (E,E)-farnesol-rich *Bothriochloa* species in South America based on Maxent models

Species	**Core suitable region(s)**	**Overlap with known distribution**	**Notes**
B. alta	Central Argentina (Pampas and surrounding regions)	High	Suitable areas largely coincide with known occurrences
B. barbinodis	Andean corridor and northwestern Argentina	High	Suitable areas largely coincide with occurrence records
B. eurylemma	Argentine Mesopotamia and adjacent regions of Uruguay and southern Brazil	Moderate	Potential expansion of suitable habitat into Uruguay beyond current occurrence records
B. imperatoides	Argentine Mesopotamia and Uruguay	High	Suitable habitat mainly restricted to northeastern Argentina and Uruguay
B. laguroides	Southern Brazil-Uruguay-central Argentina corridor	High	Suitable habitat concentrated along the southern Brazil-Uruguay-central Argentina corridor
B. longipaniculata	Northeast Argentina, Paraguay and southwest Brazil	High	Suitable areas largely coincide with known occurrences
B. meridionalis	Northeastern Argentina and southern Brazil	High	Suitable areas largely coincide with known occurrences
B. perforata	Central Argentina	High	Suitable habitat closely matches known occurrence records
B. saccharoides subsp. *australis*	Broad subtropical-tropical corridor	Moderate	Large predicted expansion beyond known occurrence records, particularly in southeastern Argentina
B. springfieldii	Central and northwestern Argentina	High	Predicted suitable habitat mainly restricted to central and northwestern Argentina

Discussion

The species distribution models exhibited good discriminative performance across all 10 South American *Bothriochloa* species rich in (E,E)-farnesol, indicating that the selected climatic and edaphic variables adequately capture broad-scale environmental conditions associated with their distributions. Across species, variables related to thermal stability (Bio3), atmospheric moisture (WVP), precipitation seasonality (Bio15), and soil properties (pH and bulk density) consistently emerged as influential predictors of habitat suitability across species, although their relative importance varied among taxa. This pattern underscores the joint role of macroclimatic gradients and substrate characteristics in shaping the ecological niches of these aromatic grasses.

The unimodal or broadly tolerant response shapes observed for these key predictors further support their interpretation as broad-scale environmental correlates rather than strict ecological thresholds. The predicted suitability patterns were broadly consistent with the currently documented distributions of most species. In the majority of cases, areas identified by the models as highly suitable largely overlapped with known occurrence records, suggesting that the selected environmental predictors capture major components of the ecological space occupied by these taxa. However, for some species, particularly *B. eurylemma* and *B. saccharoides* subsp. *australis*, the models also identified suitable areas beyond currently documented records. Such mismatches between predicted suitability and observed occurrences are common in species distribution modelling and may reflect incomplete sampling in some regions or differences between the potential environmental niche and the realized distribution constrained by dispersal limitation, historical factors, or biotic interactions (Guisan and Thuiller 2005; Franklin 2010; Peterson et al. 2011). These findings are consistent with previous evidence indicating that *Bothriochloa* species occupy environmentally differentiated niches across South America, shaped primarily by temperature regimes, moisture availability, and soil properties. Recent studies addressing niche divergence and polyploidy-driven biogeographic patterns within the genus have highlighted the importance of climatic variables related to thermal stability and water balance as key determinants of species distributions (Scrivanti and Anton 2025). The results extend this framework by showing that these same environmental gradients are associated with the occurrence of species characterized by high (E,E)-farnesol content, indicating a spatial correspondence between distributional patterns and the occurrence of chemically characterized species at continental scales.

At the level of chemical ecology, the prominence of thermal stability, atmospheric moisture, and precipitation seasonality as predictors of habitat suitability is consistent with experimental evidence demonstrating that terpenoid biosynthesis responds to abiotic stress gradients, particularly heat and water limitation (Gershenzon 1984; Holopainen and Gershenzon 2010; Khodadadi et al. 2023; Shan and Jin 2025). Oxygenated sesquiterpenes such as (E,E)-farnesol contribute to membrane stabilization, antioxidant defense, and protection against thermal and oxidative stress (Peñuelas and Llusià 2001; Loreto and Schnitzler 2010). However, in the present study, no direct measurements of (E,E)-farnesol content across environmental gradients were available. Therefore, the observed associations in the models should be interpreted as broad-scale spatial correlations between environmental conditions and species occurrence, while mechanistic links between environment and terpenoid biosynthesis remain hypotheses supported by the broader literature rather than demonstrated by the modeling results.

Two complementary but conceptually distinct levels of inference are therefore addressed in this study. First, the species distribution models identify environmental correlates of species occurrence, describing the climatic and edaphic conditions under which (E,E)-farnesol-rich *Bothriochloa* species are most frequently found. Second, although experimental studies suggest that environmental factors can influence terpenoid biosynthesis, the present models do not evaluate environmental drivers of (E,E)-farnesol concentration or accumulation within species. Consequently, the results should be interpreted as correlative associations between environmental conditions and the geographic occurrence of chemically characterized taxa, rather than as evidence of direct environmental regulation of secondary metabolite production.

Interspecific differences among *Bothriochloa* species further indicate that distinct combinations of climatic and edaphic factors are associated with their distributions. Species whose suitable habitats are more strongly linked to vapour pressure and precipitation seasonality tend to occur in environments characterized by fluctuating water availability, whereas species associated with soil pH and bulk density appear more constrained by substrate conditions influencing nutrient availability and root performance. These associations describe patterns of species occurrence and habitat suitability, and do not imply direct regulation of secondary metabolite biosynthesis by individual environmental variables. This interpretation is further supported by the frequent contrasts observed between percent contribution and permutation importance, indicating that several predictors capture overlapping dimensions of environmental variation rather than acting as independent drivers. Comparable interactions between climate, soil properties, and secondary metabolism have been documented in other aromatic grasses and terpene-rich taxa, supporting the view that multiple environmental dimensions jointly structure both species distributions and chemical profiles (Blanch et al. 2007; Haberstroh et al. 2018; Mishra et al. 2025; Zhao et al. 2025).

Similar ecological-chemical associations have been reported across plant lineages. For instance, chemotypic variation correlated with climatic gradients has been described in *Eucalyptus*, while shifts in terpene composition under water-deficit stress have been demonstrated in *Thymus* and other aromatic taxa (Bustos-Segura 2017; Mahdavi et al. 2020). Together, these studies reinforce the interpretation that environmental gradients may be correlated with spatial differentiation in secondary metabolite profiles, even though such relationships may arise through multiple indirect ecological mechanisms. Beyond their ecological relevance, these patterns have applied implications. Given the documented antimicrobial, anti-inflammatory, anticancer, and anti-biofilm activities of (E,E)-farnesol, identifying environmental conditions associated with the occurrence of (E,E)-farnesol-rich species may help guide future research on medicinally valuable grasses. However, it is important to distinguish between identifying environmental contexts where these species occur and identifying locations where metabolite production may be highest. The present models address the former by describing the climatic and edaphic environments associated with species distributions, but they do not predict spatial variation in (E,E)-farnesol concentration or yield. Consequently, the suitability maps should be interpreted as indicators of potential occurrence rather than as predictors of metabolite abundance. Within this framework, the results may still provide a useful first step for guiding conservation planning, targeted field surveys, and future bioprospecting efforts that incorporate direct chemical analyses. In contrast to previous floristic, phytochemical, and biogeographical studies on *Bothriochloa*, this study explicitly links the continental-scale distribution of (E,E)-farnesol-rich species with quantified environmental correlates. Earlier work has largely focused on taxonomy, regional floristics, or species-level chemical composition without integrating these dimensions into a spatially explicit environmental framework. By combining species distribution modeling with climatic and edaphic predictors, this study provides the first comparative, continent-wide assessment of how environmental gradients are associated with the occurrence of (E,E)-farnesol-rich *Bothriochloa* species across South America.

From a biogeographical and applied perspective, the results indicate that species characterized by high (E,E)-farnesol content are associated with environmentally differentiated suitability patterns structured along gradients of temperature stability, moisture availability, and soil alkalinity. Although future climatic scenarios were not explicitly modelled, changes in temperature and moisture regimes may contextually affect the spatial availability of suitable habitats, potentially increasing vulnerability in species with restricted distributions such as *B. alta* and *B. perforata*. Identifying areas of high climatic suitability for medicinally valuable plants, therefore, provides a useful framework for conservation planning and the sustainable use of pharmacologically relevant species (Shrestha et al. 2022; Wani et al. 2024).

Despite the robust performance of the models, several limitations should be acknowledged. It is important to note that model performance metrics, such as AUC, and variable contributions, are context-dependent; the use of a broad continental background extent may yield higher accuracy values, but it provides a robust framework for interspecific comparison. Because a common continental background was used, the models reflect relative suitability within a broad environmental space rather than species-specific dispersal constraints, and results should be interpreted accordingly. A potential source of uncertainty in species distribution modelling is the definition of background extent and the selection of model parameterization, particularly when occurrence sample sizes are limited. To evaluate the robustness of the models, a sensitivity analysis was conducted testing alternative background extents and regularization settings for species with relatively few occurrence records. The resulting models showed broadly consistent suitability patterns and similar rankings of the most influential environmental predictors, indicating that the main conclusions are not strongly dependent on specific modelling settings (Table 3).

For species with low numbers of occurrence records, the relatively high number of environmental predictors retained after correlation filtering may increase model complexity and uncertainty, potentially leading to overfitting and unstable estimates of variable importance; therefore, these models were intentionally interpreted as exploratory representations of broad-scale environmental associations rather than as optimized predictive tools, prioritizing methodological consistency across taxa and comparative inference at the continental scale. In addition, the spatial resolution of climatic (~5 km) and edaphic (~1 km) layers may not fully capture fine-scale microenvironmental heterogeneity relevant to perennial grasses. Occurrence records compiled from herbaria and online databases may introduce spatial sampling biases. Moreover, environmental variables were used as proxies for ecological conditions potentially associated with the occurrence of (E,E)-farnesol, but the models do not account for temporal variation in essential oil composition, phenological stage, or local biotic interactions. Consequently, the associations identified here should be interpreted as broad-scale correlative patterns rather than direct causal relationships.

Overall, the results indicate that macroclimatic and soil gradients jointly structure the ecological niches of (E,E)-farnesol-rich *Bothriochloa* species, providing biogeographical context for understanding the spatial distribution of chemical specialization in this genus. Future studies integrating fine-scale environmental data, seasonal chemical analyses, and experimental approaches will be essential to elucidate the mechanisms linking environmental gradients, species distributions, and terpenoid biosynthesis.

In conclusion, this study provides a continent-wide assessment of the climatic and edaphic gradients associated with the distribution of South American *Bothriochloa* species characterized by high (E,E)-farnesol content. Rather than reflecting the influence of a single controlling factor, species occurrences are associated with combinations of thermal stability, moisture regimes, precipitation seasonality, and soil properties, underscoring the multidimensional nature of environmental filtering in aromatic grasses. Across species, isothermality (Bio3), precipitation seasonality (Bio15), and atmospheric moisture (WVP), together with edaphic variables such as soil pH and bulk density (BDOD) were among the environmental correlates most frequently associated with habitat suitability. These predictors should be interpreted as broad-scale environmental correlates of species occurrence rather than direct drivers of secondary metabolite production. From biogeographical perspective, these patterns indicate that (E,E)-farnesol-rich species occupy the same broad environmental gradients that structure *Bothriochloa* distributions at continental scales. The observed association between niche differentiation and the geographic occurrence of (E,E)-farnesol-rich species indicates that environmental heterogeneity across South America provides a spatial framework in which ecological and chemical diversity are jointly maintained. As demonstrated by the response curves and variable importance patterns, these associations reflect broad-scale correlative relationships rather than direct environmental controls. Beyond their ecological relevance, these insights have applied implications for the conservation and sustainable use of phytochemical diversity. Identifying environmental contexts associated with (E,E)-farnesol-rich species helps to prioritize regions where both biodiversity and chemically valuable traits may be particularly sensitive to ongoing climatic changes.

ACKNOWLEDGEMENTS

I am grateful to the curators of the following herbaria for their generosity in arranging specimen loans: AU, B, CEN, CGMS, COL, CORD, F, ICN, MO, NY, S, SI, SP, U, and US. This work was supported by Universidad Nacional de Córdoba, Argentina (SECyT-UNC Res 266/23 PIDTA).

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