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Detailed description of methods used in species distribution modelling of *Aspalathus linearis*

Modelling approach

MaxEnt is a machine learning algorithm used for modelling species distributions. It predicts the relative suitability (0 to 1) for a species' occurrence across a landscape based on environmental predictor variables.[1] MaxEnt works by finding the probability distribution of maximum entropy (i.e. the most spread out or least constrained distribution) that matches the constraints imposed by the environmental variables and known species occurrences.[2] MaxEnt is among the best performing species distribution modelling methods and has been widely used in ecology, conservation biology, and biogeography to predict species distributions and habitat suitability under current and future environmental conditions.[3,4]

Although MaxEnt generally performs well for modelling species distributions, a few model choices and parameter settings can affect model outputs.[5] We therefore used an ensemble modelling approach to capture model uncertainty[6] in which 100 models were run for each ecotype (including the species as a whole), with settings determined by a Sobol sampling process that allowed for uniform sample values or options from across the full range of model settings (explained below; see Convertino et al.[7] for a similar approach). The MaxEnt settings of interest that were sampled, as described above, were as follows: (i) the number of pseudo-absences selected within the study area, ranging from twice the number of occurrences to 20 000[8]; (ii) the MaxEnt regularisation parameter, which we allowed to vary from 1 to 5[5]; (iii) MaxEnt features – linear (L), quadratic (Q), and product (P), with a choice allowed from the combinations, LQ, LP, QP or LQP[5]. To conduct the Sobol sampling across the continuum of parameter specifications described above, we used the parameterSets function from the R package *sensitivity* to generate 100 different model setting combinations.

Occurrences

The data collected to determine the current occurrence of the species and ecotypes were used as input data for the models. These data comprised a total of 126 field-verified location records for wild rooibos, representing the four different ecotypes (Figure 1). After removing duplicate occurrences within individual pixels of the ~1 km resolution environmental predictor rasters (see section below), we were left with 100 occurrences. For modelling potential distributions, we used all 100 occurrences to model rooibos as a species in its entirety, including 12 occurrences for the Bush ecotype, 42 for the Prostrate ecotype, 33 for the Erect type, and 13 for the Salignus type (Supplementary figure 2).

Environmental predictors

We based our selection of potential predictor variables for the distribution of rooibos and its ecotypes on Lötter and Le Maitre[9], who investigated the potential distribution of rooibos under contemporary and future climate conditions. Climate variables, including total summer and winter rainfall, and maximum summer and minimum winter temperatures were argued to be the main factors affecting the distribution of this species.[9] From the CHELSA high resolution (30 arcsec, ~1 km) data set (https://chelsa-climate.org/), we used four bioclimatic variables: Precipitation of Warmest Quarter (BIO18), Precipitation of Coldest Quarter (BIO19), Maximum Temperature of Warmest Month (BIO5), and Minimum Temperature of Coldest Month. Topographical and soil factors are other potentially important factors affecting rooibos distribution.[9,10] We derived topographical slope for the study region using the ~30 m NASADEM digital elevation model and aggregated this to the same ~1 km resolution as the climate data. We used seven soil chemical layers from a data set developed specifically for the Cape Floristic region which included: soil electrical conductivity, K, Na, P, C, N, and pH.[11] Three layers representing soil structural properties, clay, silt and sand percentages, were obtained from the 250 m resolution global ISRIC SoilGrids data set (https://soilgrids.org/). We calculated the percentage clay, silt and sand for the top 15 cm of the soil profile from the top two soil layers available from SoilGrids, i.e. 0–5 cm and 5–15 cm. From these 15 potential environmental predictors, we selected 13 that were not strongly correlated with one another ($r < |0.8|$), dropping percentage clay and silt.

Model evaluation

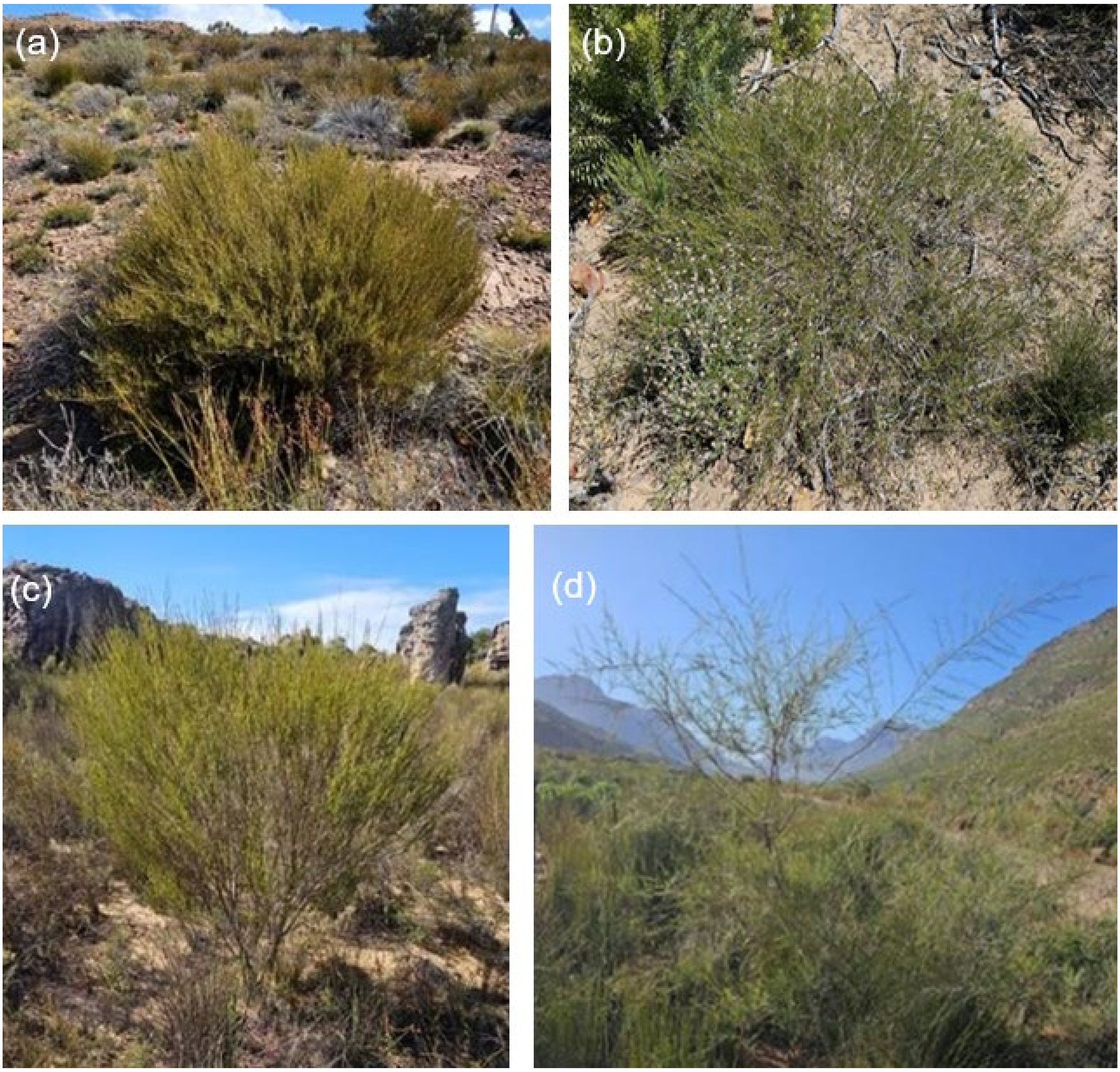
All models were evaluated using the mean area under the receiver operating characteristic curve (AUC). For the species as a whole (all ecotypes together), model evaluation was done using five environmentally separated folds using the R package *blockCV,* i.e. 80% of the data were used for model training and 20% for testing, with each fold being used for testing.[12] For rooibos ecotypes, models were evaluated using a jackknife approach, i.e. each occurrence was used in turn for testing a model trained using all remaining other occurrences. A jackknife approach was used in these instances because ecotypes generally had relatively low numbers of occurrences (all <42).[13,14]

Predicted distributions

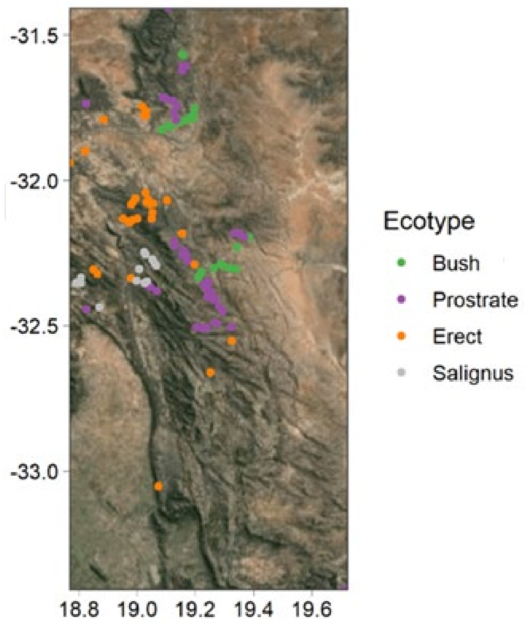
For each model, we predicted the distribution of rooibos as a species in its entirety or of individual ecotypes using the *cloglog* output of MaxEnt, which can be interpreted as a measure of relative environmental suitability.[1] Using the 100 model outputs for each ecotype, we created a weighted predicted suitability map by multiplying each model run predicted distribution by its respective AUC value, and thereafter calculating a weighted mean suitability. To enable simpler comparison of model outputs, we transformed the relative suitability maps to binary presence/absence predictions using a threshold value equivalent to the maximum sum of sensitivity and specificity.[15] Both the suitability and binary predictions were masked by multivariate environmental similarity surface (MESS) values less than zero – these are areas where the models are extrapolating into novel environmental space.[2]

Environmental correlates of distribution

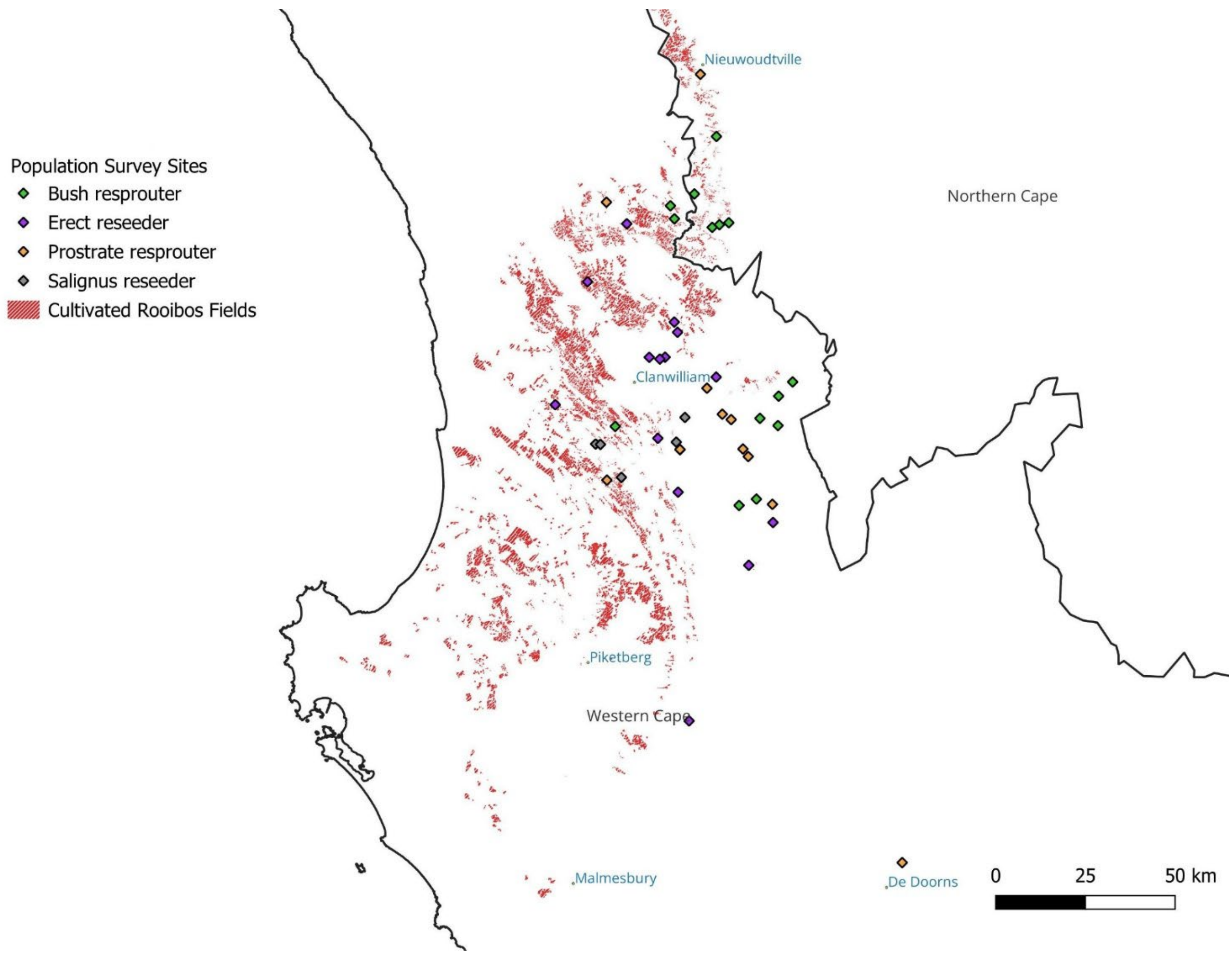
To investigate environmental factors that potentially affect the distribution of rooibos and its ecotypes, we produced response curves illustrating the relationship between each environmental predictor and the predicted relative suitability. Outputs from each of the 100 model runs were plotted, as well as a weighted mean response which was calculated by multiplying suitability values by the respective AUC value for each model run. The output from the model with the best (highest) AUC value was also highlighted on these plots.



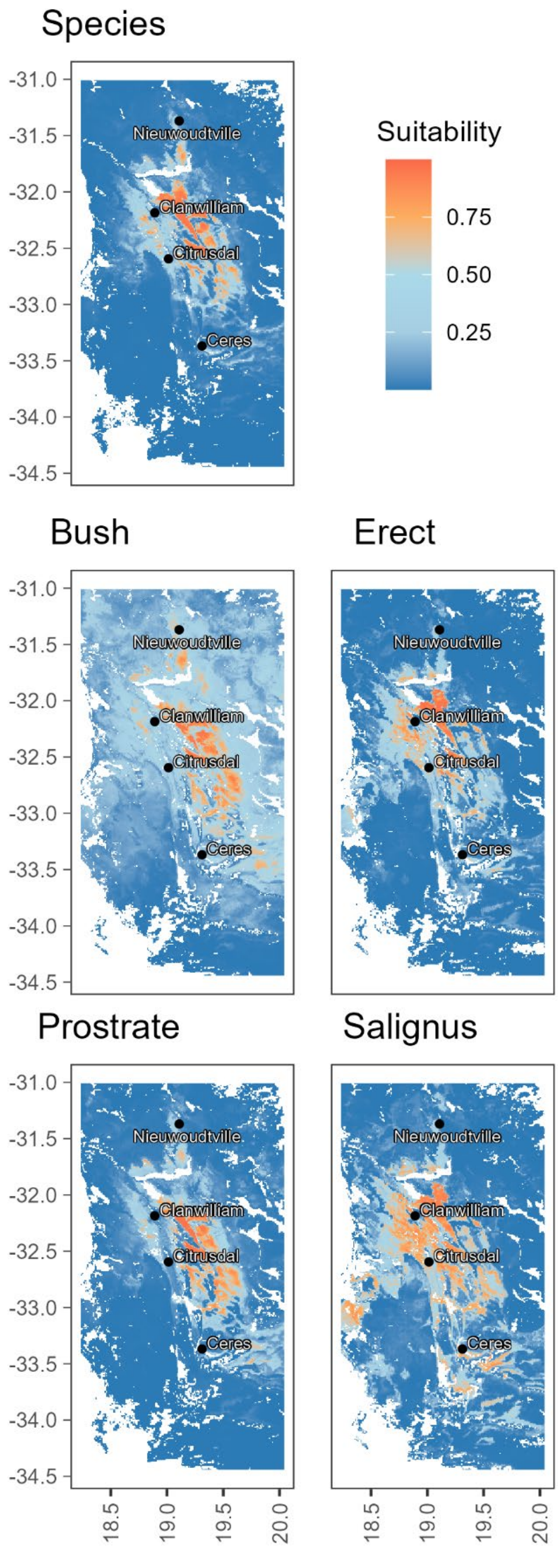
Supplementary figure 1: Exemplary images of the different ecotypes or growth forms of wild rooibos (*Aspalathus linearis*), namely the (a) Bush or Shrub form, (b) Prostrate form, (c) Erect (including Upright or Tree) form, and (d) Salignus form.



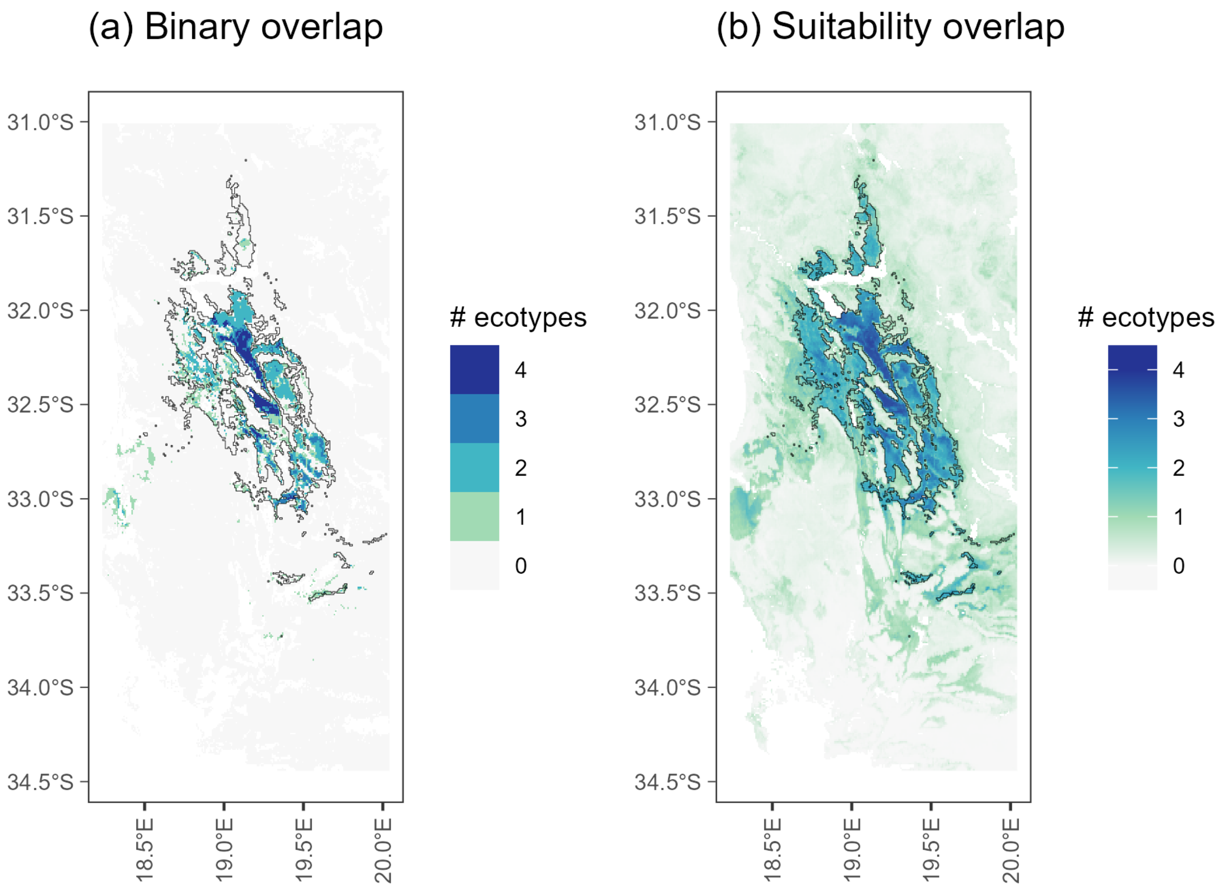
Supplementary figure 2: Field-verified location records of the four wild rooibos ecotypes used for MaxEnt modelling.



Supplementary figure 3: Distribution of cultivated rooibos fields in relation to the predicted (modelled) distribution of wild rooibos and the locations of population survey sites.

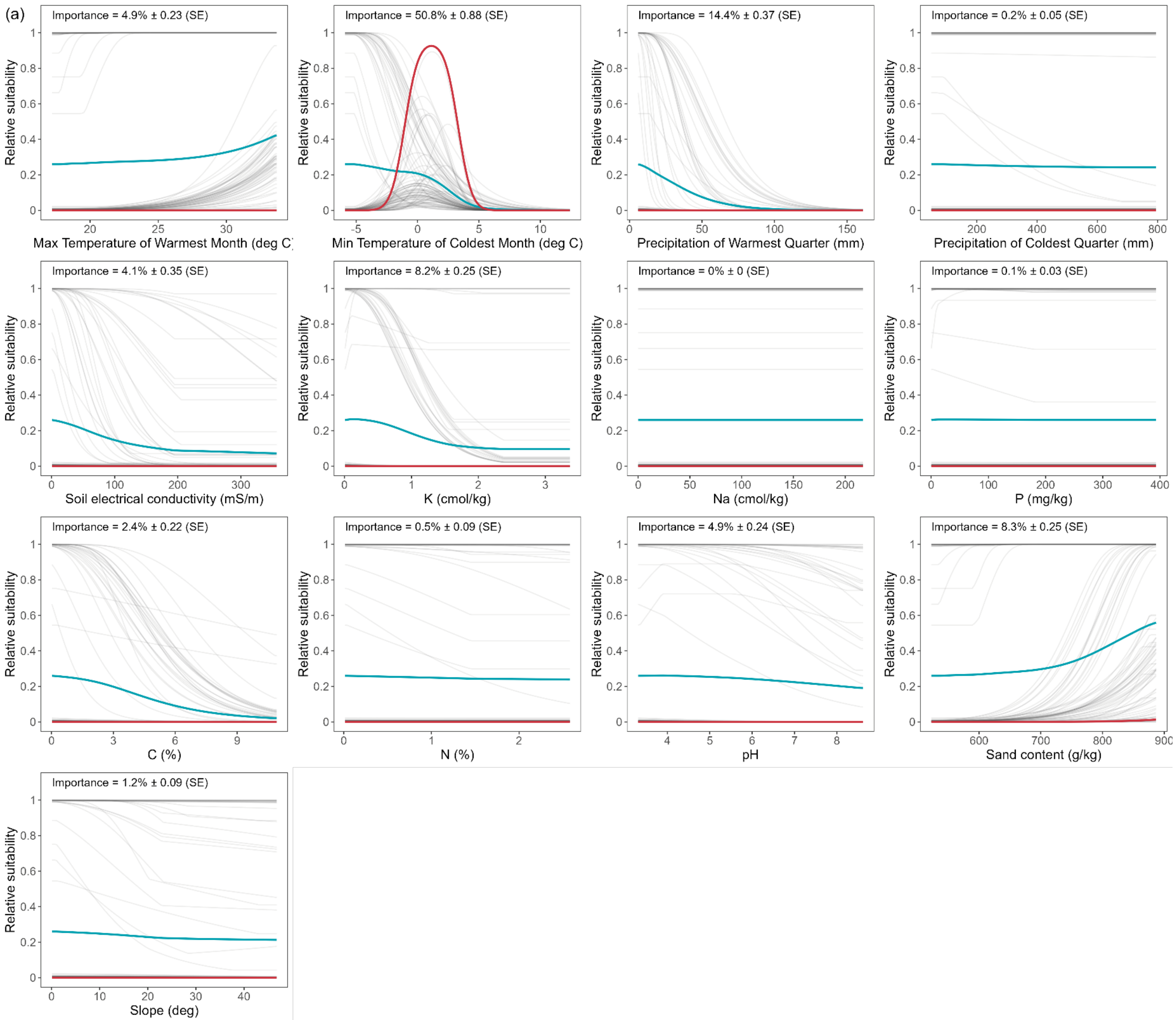


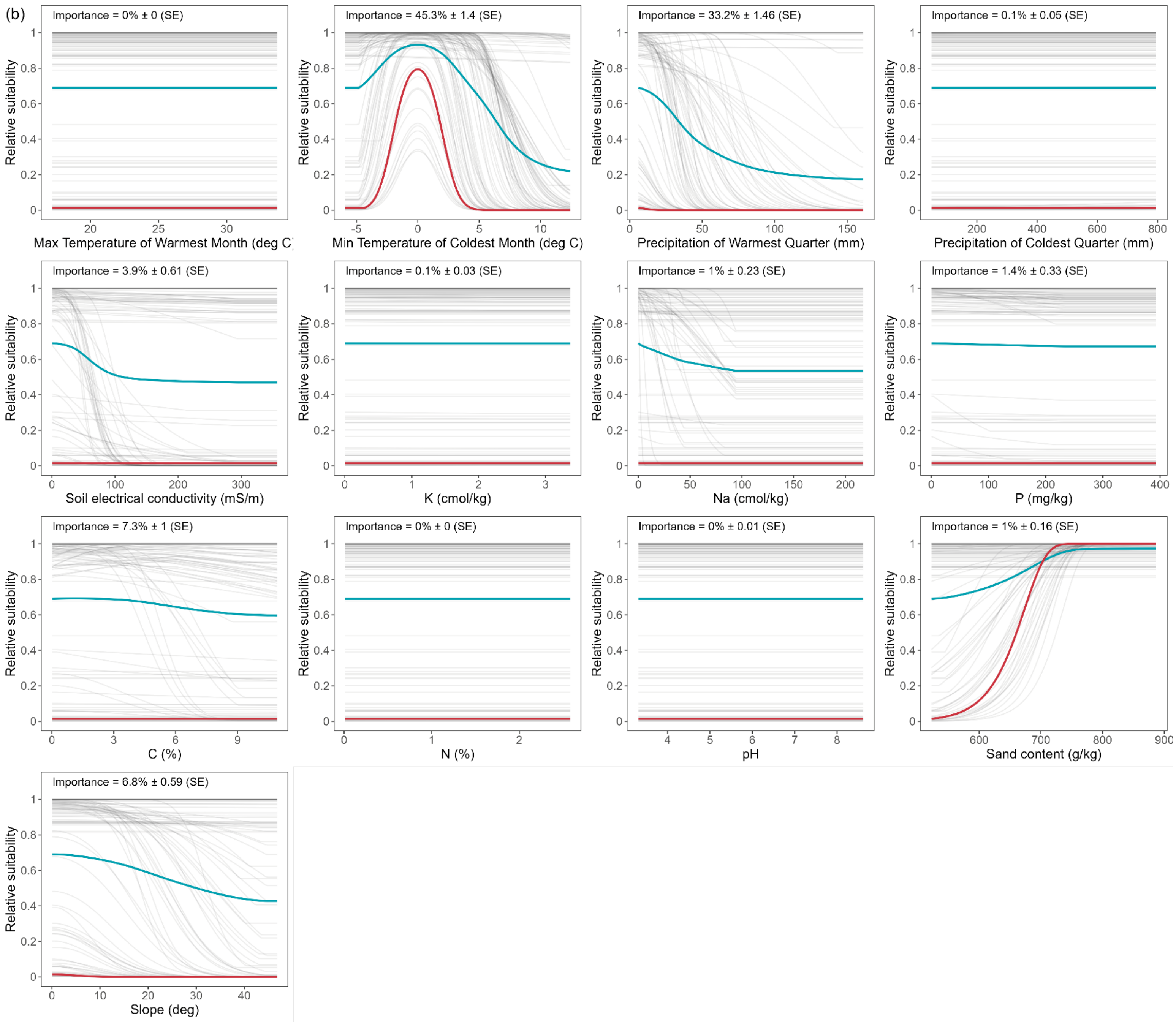
Supplementary figure 4: Predicted distributions of wild *Aspalathus linearis* for the species as a whole (Species) and for each of the four ecotypes (Bush, Erect, Prostrate, Salignus). Distributions are based on predicted suitability values, with red indicating high suitability and blue indicating low suitability.

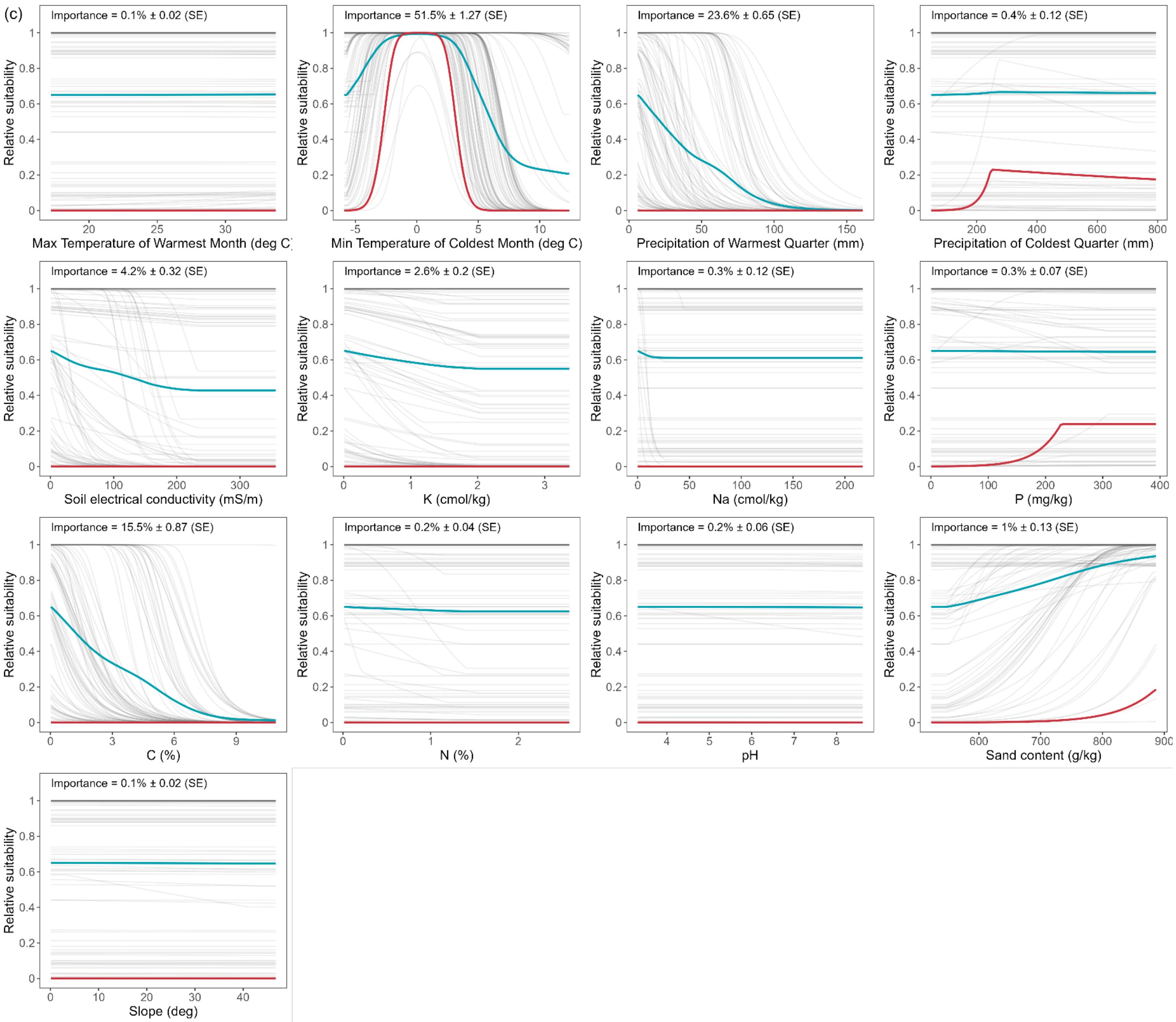


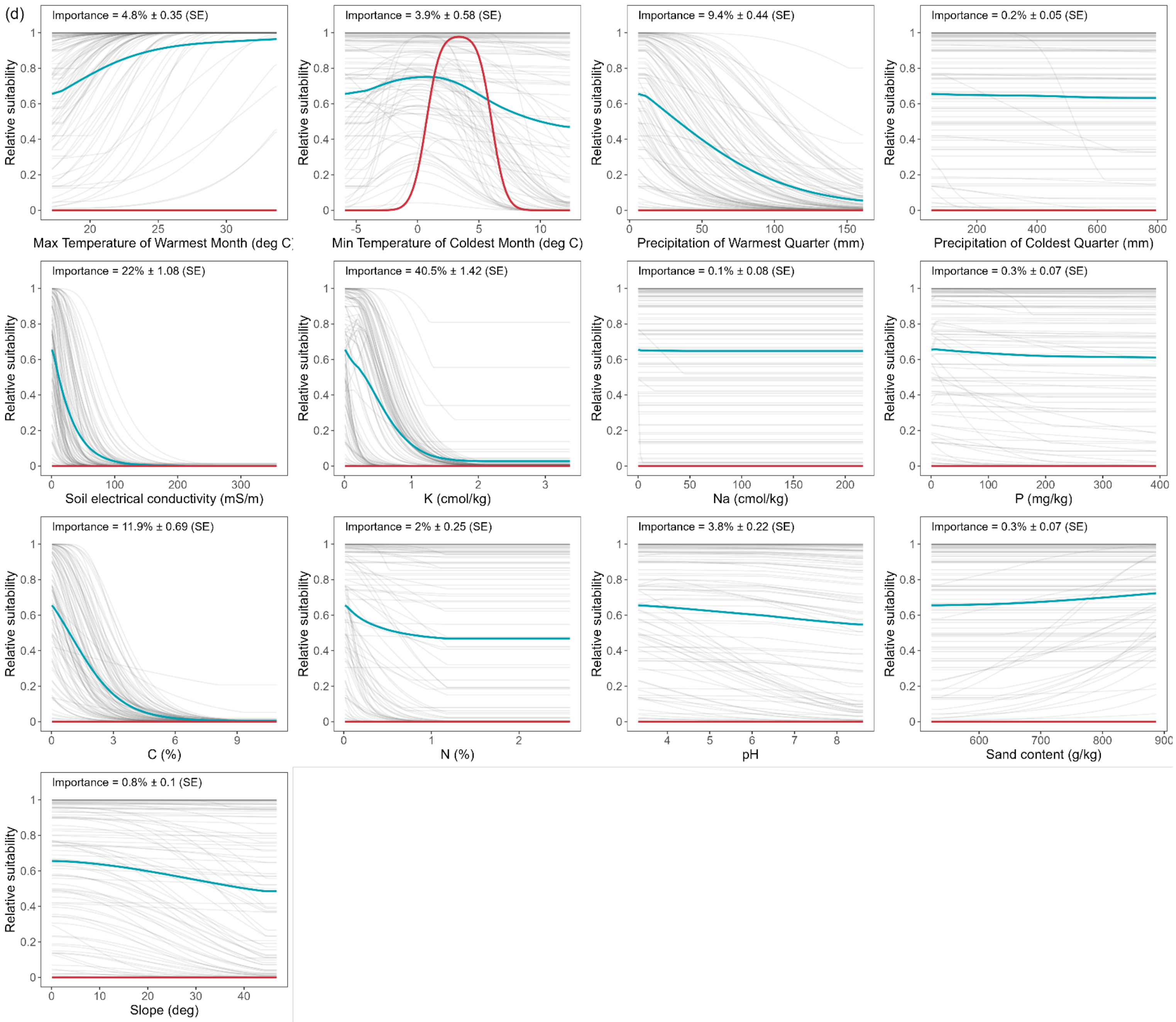
Supplementary figure 5: Overlap of predicted rooibos ecotype distributions expressed as the sum of the number of ecotypes predicted to occur in any given pixel (max = 4 in blue). (a) The sum of binary (presence/absence) predictions. (b) The sum of suitability values. The predicted distribution of the species as a whole is indicated by the area within the grey polygons. This highlights the generally distinct distributions of each ecotype except for the core of the species as a whole.

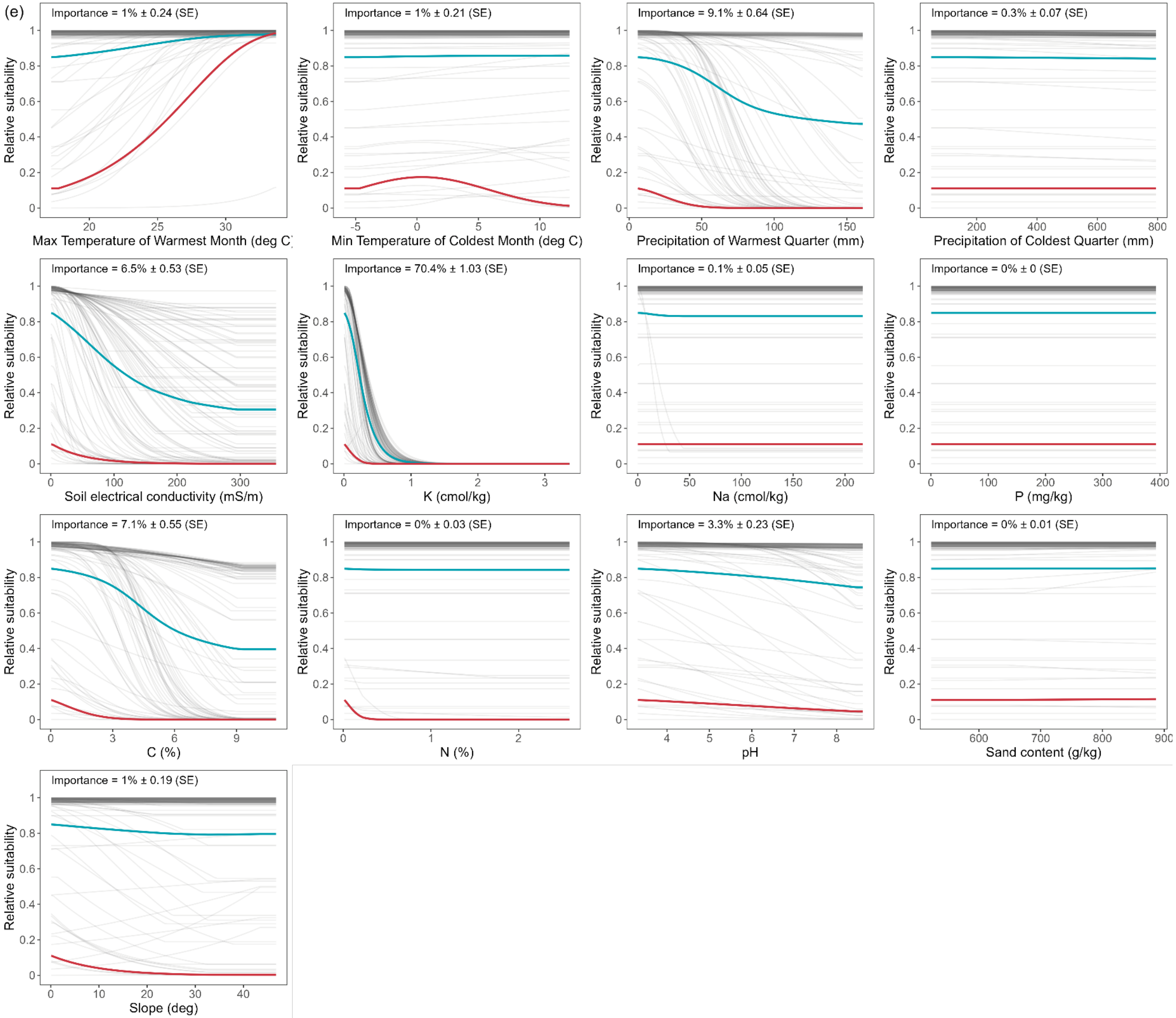
Supplementary figure 6 [below]: Response curves showing the relationship between predicted suitability for **(a) rooibos** as a species, and the respective ecotypes **(b) Bush**, **(c) Prostrate**, **(d) Erect**, and **(e) Salignus** and each of the 13 environmental variables used as model predictors. Grey lines represent individual model runs, the blue line the weighted mean of all 100 model runs and the red line is the best model (highest AUC value). Mean variable importance (and standard error) is shown above each variable.


(a)
Importance = 4.9% ± 0.23 (SE)
Max Temperature of Warmest Month (deg C)
Importance = 50.8% ± 0.88 (SE)
Min Temperature of Coldest Month (deg C)
Importance = 14.4% ± 0.37 (SE)
Precipitation of Warmest Quarter (mm)
Importance = 0.2% ± 0.05 (SE)
Precipitation of Coldest Quarter (mm)
Importance = 4.1% ± 0.35 (SE)
Soil electrical conductivity (mS/m)
Importance = 8.2% ± 0.25 (SE)
K (cmol/kg)
Importance = 0% ± 0 (SE)
Na (cmol/kg)
Importance = 0.1% ± 0.03 (SE)
P (mg/kg)
Importance = 2.4% ± 0.22 (SE)
C (%)
Importance = 0.5% ± 0.09 (SE)
N (%)
Importance = 4.9% ± 0.24 (SE)
pH
Importance = 8.3% ± 0.25 (SE)
Sand content (g/kg)
Importance = 1.2% ± 0.09 (SE)
Slope (deg)
Relative suitability


(b)
Importance = 0% ± 0 (SE)
Max Temperature of Warmest Month (deg C)
Importance = 45.3% ± 1.4 (SE)
Min Temperature of Coldest Month (deg C)
Importance = 33.2% ± 1.46 (SE)
Precipitation of Warmest Quarter (mm)
Importance = 0.1% ± 0.05 (SE)
Precipitation of Coldest Quarter (mm)
Importance = 3.9% ± 0.61 (SE)
Soil electrical conductivity (mS/m)
Importance = 0.1% ± 0.03 (SE)
K (cmol/kg)
Importance = 1% ± 0.23 (SE)
Na (cmol/kg)
Importance = 1.4% ± 0.33 (SE)
P (mg/kg)
Importance = 7.3% ± 1 (SE)
C (%)
Importance = 0% ± 0 (SE)
N (%)
Importance = 0% ± 0.01 (SE)
pH
Importance = 1% ± 0.16 (SE)
Sand content (g/kg)
Importance = 6.8% ± 0.59 (SE)
Slope (deg)
Relative suitability


(c)
Importance = 0.1% ± 0.02 (SE)
Max Temperature of Warmest Month (deg C)
Importance = 51.5% ± 1.27 (SE)
Min Temperature of Coldest Month (deg C)
Importance = 23.6% ± 0.65 (SE)
Precipitation of Warmest Quarter (mm)
Importance = 0.4% ± 0.12 (SE)
Precipitation of Coldest Quarter (mm)
Importance = 4.2% ± 0.32 (SE)
Soil electrical conductivity (mS/m)
Importance = 2.6% ± 0.2 (SE)
K (cmol/kg)
Importance = 0.3% ± 0.12 (SE)
Na (cmol/kg)
Importance = 0.3% ± 0.07 (SE)
P (mg/kg)
Importance = 15.5% ± 0.87 (SE)
C (%)
Importance = 0.2% ± 0.04 (SE)
N (%)
Importance = 0.2% ± 0.06 (SE)
pH
Importance = 1% ± 0.13 (SE)
Sand content (g/kg)
Importance = 0.1% ± 0.02 (SE)
Slope (deg)
Relative suitability


(d)
Importance = 4.8% ± 0.35 (SE)
Max Temperature of Warmest Month (deg C)
Importance = 3.9% ± 0.58 (SE)
Min Temperature of Coldest Month (deg C)
Importance = 9.4% ± 0.44 (SE)
Precipitation of Warmest Quarter (mm)
Importance = 0.2% ± 0.05 (SE)
Precipitation of Coldest Quarter (mm)
Importance = 22% ± 1.08 (SE)
Soil electrical conductivity (mS/m)
Importance = 40.5% ± 1.42 (SE)
K (cmol/kg)
Importance = 0.1% ± 0.08 (SE)
Na (cmol/kg)
Importance = 0.3% ± 0.07 (SE)
P (mg/kg)
Importance = 11.9% ± 0.69 (SE)
C (%)
Importance = 2% ± 0.25 (SE)
N (%)
Importance = 3.8% ± 0.22 (SE)
pH
Importance = 0.3% ± 0.07 (SE)
Sand content (g/kg)
Importance = 0.8% ± 0.1 (SE)
Slope (deg)
Relative suitability


(e)
Importance = 1% ± 0.24 (SE)
Max Temperature of Warmest Month (deg C)
Importance = 1% ± 0.21 (SE)
Min Temperature of Coldest Month (deg C)
Importance = 9.1% ± 0.64 (SE)
Precipitation of Warmest Quarter (mm)
Importance = 0.3% ± 0.07 (SE)
Precipitation of Coldest Quarter (mm)
Importance = 6.5% ± 0.53 (SE)
Soil electrical conductivity (mS/m)
Importance = 70.4% ± 1.03 (SE)
K (cmol/kg)
Importance = 0.1% ± 0.05 (SE)
Na (cmol/kg)
Importance = 0% ± 0 (SE)
P (mg/kg)
Importance = 7.1% ± 0.55 (SE)
C (%)
Importance = 0% ± 0.03 (SE)
N (%)
Importance = 3.3% ± 0.23 (SE)
pH
Importance = 0% ± 0.01 (SE)
Sand content (g/kg)
Importance = 1% ± 0.19 (SE)
Slope (deg)
Relative suitability

Supplementary table 1: Proclaimed protected areas on state (S) or private (P) land which partially occur within the predicted distribution range (Figure 2) of A*spalathus linearis* and its ecotypes

Species/ecotype	**Protected area name**	**Designation**	**State/private**	**Entire protected area (ha)**	**Area (ha) of protected area in range**
A. linearis	Sederberg Mountain Catchment Area	Mountain Catchment Area	P	59 414	33 095
A. linearis	Sederberg Wilderness Area	Forest Wilderness Area, WHS	S	62 794	32 360
A. linearis	Koue Bokkeveld Mountain Catchment Area	Mountain Catchment Area	P	96 857	17 371
A. linearis	Groenfontein Private Nature Reserve	Nature Reserve	P	14 014	13 752
A. linearis	Matjies Rivier Provincial Nature Reserve	Nature Reserve, WHS	S	18 754	10 485
A. linearis	Winterhoek Mountain Catchment Area	Mountain Catchment Area	S	51 325	8 123
A. linearis	Matroosberg Mountain Catchment Area	Mountain Catchment Area	P	82 531	5 694
A. linearis	Dwarsrivier Nature Reserve	Nature Reserve	P	5 808	5 235
A. linearis	Wagenboom Nature Reserve	Nature Reserve	P	6 467	4 629
A. linearis	Cederberg Private Nature Reserve	Nature Reserve	S	4 062	3 397
A. linearis	Oorlogskloof Nature Reserve	Nature Reserve	S	6 170	3 272
A. linearis	Mooiberg Nature Reserve	Nature Reserve	P	3 186	3 186
A. linearis	Kromrivierkloof Nature Reserve	Nature Reserve	P	3 904	2 288
A. linearis	Bakkrans Nature Reserve	Nature Reserve	P	2 288	2 204
A. linearis	Taaiboschkraal Nature Reserve	Nature Reserve	P	4 625	1 720
A. linearis	Ben Etive Nature Reserve	Nature Reserve	P	5 085	1 522
A. linearis	Alsfontein Nature Reserve	Nature Reserve	P	1 325	1 325
A. linearis	Skimmelberg Nature Reserve	Nature Reserve	P	1 353	1 299
A. linearis	Grootwinterhoek Protected Environment	Protected Environment	P	4 351	1 138
A. linearis	Vogelfontein Nature Reserve	Nature Reserve	P	1 488	1 096
A. linearis	Klein Cederberg Private Nature Reserve	Nature Reserve	P	990	990
A. linearis	Hooggelegen Nature Reserve	Nature Reserve	P	825	724
A. linearis	Nieuwe Gift Nature Reserve	Nature Reserve	P	564	552
A. linearis	Op de Berg Private Nature Reserve	Nature Reserve	P	423	423
A. linearis	Ceres Bergfynbos Reserve	Nature Reserve	P	7 000	389
A. linearis	Bergwater Private Nature Reserve	Nature Reserve	P	304	272
A. linearis	Tweekuilen Nature Reserve	Nature Reserve	P	1 335	140
A. linearis	Kruis Nature Reserve	Nature Reserve	P	323	87
A. linearis	Mountshoek Protected Environment	Protected Environment	P	7 181	72
A. linearis	Hawequas Mountain Catchment Area	Mountain Catchment Area	P	51 604	71
A. linearis	Vogelfontein 319 Nature Reserve	Nature Reserve	P	57	57
A. linearis	Banghoek Private Nature Reserve	Nature Reserve	P	1 035	20
A. linearis	Rondeberg Oord Private Nature Reserve	Nature Reserve	P	266	18

Species/ecotype	Protected area name	Designation	State/private	Entire protected area (ha)	Area (ha) of protected area in range
Bush	Sederberg Wilderness Area	Forest Wilderness Area, WHS	S	62 794	7 308
Bush	Groenfontein Private Nature Reserve	Nature Reserve	P	14 014	5 060
Bush	Matjies Rivier Provincial Nature Reserve	Nature Reserve, WHS	S	18 754	4 376
Bush	Dwarsrivier Nature Reserve	Nature Reserve	P	5 808	4 346
Bush	Cederberg Private Nature Reserve	Nature Reserve	P	4 062	3 272
Bush	Koue Bokkeveld Mountain Catchment Area	Mountain Catchment Area	P	96 857	1 847
Bush	Mooiberg Nature Reserve	Nature Reserve	P	3 186	1 741
Bush	Kromrivierkloof Nature Reserve	Nature Reserve	P	3 904	1 440
Bush	Bakkrans Nature Reserve	Nature Reserve	P	2 288	1 344
Bush	Wagenboom Nature Reserve	Nature Reserve	P	6 467	1 096
Bush	Klein Cederberg Private Nature Reserve	Nature Reserve	P	990	722
Bush	Alsfontein Nature Reserve	Nature Reserve	P	1 325	324
Bush	Vogelfontein Nature Reserve	Nature Reserve	P	1 488	255
Bush	Op de Berg Private Nature Reserve	Nature Reserve	P	423	170
Bush	Oorlogskloof Nature Reserve	Nature Reserve	S	6 170	146
Bush	Sederberg Mountain Catchment Area	Mountain Catchment Area	S	59 414	127
Bush	Matroosberg Mountain Catchment Area	Mountain Catchment Area	P	82 531	42
Bush	Bergwater Private Nature Reserve	Nature Reserve	P	304	25
Prostrate	Sederberg Wilderness Area	Forest Wilderness Area, WHS	S	62 794	13 547
Prostrate	Sederberg Mountain Catchment Area	Mountain Catchment Area	P	59 414	7 661
Prostrate	Groenfontein Private Nature Reserve	Nature Reserve	P	14 014	6 843
Prostrate	Koue Bokkeveld Mountain Catchment Area	Mountain Catchment Area	P	96 857	6 323
Prostrate	Matjies Rivier Provincial Nature Reserve	Nature Reserve, WHS	S	18 754	5 734
Prostrate	Dwarsrivier Nature Reserve	Nature Reserve	P	5 808	4 984
Prostrate	Cederberg Private Nature Reserve	Nature Reserve	P	4 062	2 590
Prostrate	Mooiberg Nature Reserve	Nature Reserve	P	3 186	2 241
Prostrate	Bakkrans Nature Reserve	Nature Reserve	P	2 288	2 110
Prostrate	Kromrivierkloof Nature Reserve	Nature Reserve	P	3 904	1 860
Prostrate	Matroosberg Mountain Catchment Area	Mountain Catchment Area	P	82 531	1 612
Prostrate	Alsfontein Nature Reserve	Nature Reserve	P	1 325	1 325
Prostrate	Wagenboom Nature Reserve	Nature Reserve	P	6 467	1 186
Prostrate	Vogelfontein Nature Reserve	Nature Reserve	P	1 488	905
Prostrate	Klein Cederberg Private Nature Reserve	Nature Reserve	P	990	678
Prostrate	Skimmelberg Nature Reserve	Nature Reserve	P	1 353	606
Prostrate	Op de Berg Private Nature Reserve	Nature Reserve	P	423	402

Species/ecotype	Protected area name	Designation	State/private	Entire protected area (ha)	Area (ha) of protected area in range
Prostrate	Bergwater Private Nature Reserve	Nature Reserve	P	304	200
Prostrate	Nieuwe Gift Nature Reserve	Nature Reserve	P	564	185
Prostrate	Taaiboschkraal Nature Reserve	Nature Reserve	P	4 625	82
Prostrate	Winterhoek Mountain Catchment Area	Mountain Catchment Area	P	51 325	72
Prostrate	Vogelfontein 319 Nature Reserve	Nature Reserve	P	57	57
Prostrate	Hooggelegen Nature Reserve	Nature Reserve	P	825	28
Erect	Sederberg Wilderness Area	Forest Wilderness Area, WHS	S	62 794	11 832
Erect	Dwarsrivier Nature Reserve	Nature Reserve	P	5 808	4 075
Erect	Sederberg Mountain Catchment Area	Mountain Catchment Area	P	59 414	3 375
Erect	Matjies Rivier Provincial Nature Reserve	Nature Reserve, WHS	S	18 754	1 549
Erect	Koue Bokkeveld Mountain Catchment Area	Mountain Catchment Area	P	96 857	1 125
Erect	Kromrivierkloof Nature Reserve	Nature Reserve	P	3 904	982
Erect	West Coast National Park	National Park	S	36 566	236
Erect	Skimmelberg Nature Reserve	Nature Reserve	P	1 353	229
Erect	Vogelfontein Nature Reserve	Nature Reserve	P	1 488	159
Erect	Alsfontein Nature Reserve	Nature Reserve	P	1 325	158
Erect	Bergwater Private Nature Reserve	Nature Reserve	P	304	146
Erect	Winterhoek Mountain Catchment Area	Mountain Catchment Area	P	51 325	100
Erect	Rondeberg Oord Private Nature Reserve	Nature Reserve	P	266	82
Erect	Matroosberg Mountain Catchment Area	Mountain Catchment Area	P	82 531	39
Erect	Vogelfontein 319 Nature Reserve	Nature Reserve	P	57	34
Erect	Wagenboom Nature Reserve	Nature Reserve	P	6 467	7
Salignus	Sederberg Wilderness Area	Forest Wilderness Area, WHS		62 794	25 337
Salignus	Sederberg Mountain Catchment Area	Mountain Catchment Area	P	59 414	11 955
Salignus	Koue Bokkeveld Mountain Catchment Area	Mountain Catchment Area	P	96 857	8 516
Salignus	Matroosberg Mountain Catchment Area	Mountain Catchment Area	P	82 531	8 290
Salignus	Dwarsrivier Nature Reserve	Nature Reserve	P	5 808	4 857
Salignus	Winterhoek Mountain Catchment Area	Mountain Catchment Area	P	51 325	3 664
Salignus	Hawequas Mountain Catchment Area	Mountain Catchment Area	P	51 604	3 264
Salignus	Groenfontein Private Nature Reserve	Nature Reserve	P	14 014	3 150
Salignus	Grootwinterhoek Protected Environment	Protected Environment	P	4 351	2 384
Salignus	Wagenboom Nature Reserve	Nature Reserve	P	6 467	2 144
Salignus	Matjies Rivier Provincial Nature Reserve	Nature Reserve, WHS	S	18 754	2 021
Salignus	Kromrivierkloof Nature Reserve	Nature Reserve	P	3 904	2 012
Salignus	West Coast National Park	National Park	S	36 566	1 170

Species/ecotype	Protected area name	Designation	State/private	Entire protected area (ha)	Area (ha) of protected area in range
Salignus	Skimmelberg Nature Reserve	Nature Reserve	P	1 353	1 132
Salignus	Ben Etive Nature Reserve	Nature Reserve	P	5 085	913
Salignus	Ceres Bergfynbos Reserve	Nature Reserve	P	7 000	900
Salignus	Hopefield Private Nature Reserve	Nature Reserve	P	1 706	358
Salignus	Klein Cederberg Private Nature Reserve	Nature Reserve	P	990	259
Salignus	Groot-Winterhoek Wilderness Area	Forest Wilderness Area, WHS	S	24 311	216
Salignus	Bergwater Private Nature Reserve	Nature Reserve	P	304	200
Salignus	Alsfontein Nature Reserve	Nature Reserve	P	1 325	183
Salignus	Vogelfontein Nature Reserve	Nature Reserve	P	1 488	151
Salignus	Jakkalsfontein Private Nature Reserve	Nature Reserve	P	1 783	140
Salignus	Langeberg-Wes Mountain Catchment Area	Mountain Catchment Area	P	63 585	119
Salignus	Rondeberg Oord Private Nature Reserve	Nature Reserve	P	266	82

Protected areas source: https://portal.environment.gov.za/PortalDownloads/PACA_Gazettes/PA

WHS=World Heritage Site

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