

12 **SUPPLEMENTARY MATERIAL AND METHODS**

13 **(a) *Anomodont phylogeny***

14 As one of the most successful radiations of therapsid (stem-group mammal) amniotes, anomodonts
15 provide an excellent case study for exploring macroevolutionary patterns in terrestrial vertebrates
16 during a major extinction event. There has been considerable interest in the phylogeny of this group
17 over the past decade [1-10]. The analysis of anomodont interrelationships from [11], rooted on the
18 genus *Biseridens* [9], offers the most up-to-date account of the published characters, their codings
19 and formulation, and the rationale behind character-state delimitations. Our work represents the first
20 example of a disparity analysis applied to a cladistic data matrix that includes both continuous and
21 discrete characters.

22

23 **(b) *Anomodont stratigraphy***

24 The stratigraphic framework used in this study is based on J. F.'s [12] review of anomodont-bearing
25 tetrapod faunas, which used the well-established Permian-Triassic assemblage zones (AZ) from the
26 South African Karoo Basin [13], the international marine stages of the current Geologic Time Scale
27 (Standard Global Chronostratigraphic Scale; SGCS) [14], as well as the Permian and Triassic land-
28 vertebrate faunachrons (LVFs; [15-21]). Changes to absolute ages of stage boundaries, specifically
29 in the Triassic but also with respect to the Permian stages and to the chronological delimitation of
30 the Permo-Triassic boundary (PTB), adopted from [22-24]), were already implemented in the study
31 in [12] and are also employed here. In general, correlations of the Permian faunas primarily follow
32 compendia in [18,25], whereas correlations of the Triassic faunas are chiefly based on Battail [26]
33 and Lucas [15,26-28]. The rationale and details of the correlations of these faunas are discussed in
34 detail in [12] and will not be repeated here. However, the present study further considers the most
35 recent advances in the correlation schemes for southern and eastern Africa, namely those for the
36 Upper Permian Upper Madumabisa Mudstone (best known from the Luangwa Basin in Zambia)

37 and the Tanzanian Usili Formation (Ruhuhu Basin), which are now both considered to be best
38 correlated with the *Cistecephalus* Assemblage Zone of the South African Karoo Basin [29].

39

40 (c) *Disparity analyses*

41 We adopted standard protocols [30-32] to calculate character-based disparity (i.e., the amount of
42 morphological dissimilarity measured between or within groups of taxa) from the data matrix in
43 [11]. These were discussed in detail, implemented, and refined methodologically in [32-37], and
44 have been applied to numerous fossil vertebrate groups in recent years [38-47]. Although detailed
45 discussions of these protocols are available and have been extensively dealt with in various papers
46 [32,38,40], we consider it necessary to provide a very short summary and add some clarifications.
47 This is because character-based disparity analyses are less well known than those based on either
48 traditional or geometric morphometric methods. Some issues, such as inclusion of autapomorphies
49 and their impact on profiles of disparity and patterns of morphospace occupation, were addressed
50 briefly in [40,41,46] (but see also below). Others, such as the geometric interpretation of the results,
51 were discussed in [32,40]. However, we review both issues concisely here.

52 We consider character-based analyses of disparity in the context of measuring phenotypic
53 dissimilarity [48-50]. Although much research on disparity focuses on biological shape and shape
54 differences among organisms and/or their parts [51,52], we emphasize that there is no unique way
55 to measure the morphological distinctiveness of organisms. Several researchers advocate using
56 techniques for analyzing shape variation that rely solely on geometric properties of the objects (taxa
57 or their constituent parts) being measured [49,53-57]. These techniques are employed in traditional
58 (e.g., based on linear and other continuous measurements) and geometric (e.g., based on landmarks)
59 morphometrics [58-63]. These methods permit a relatively intuitive representation of specimens or
60 taxa in a multivariate morphospace in which the distances between specimens or taxa correspond to
61 the magnitude of their shape differences. Geometric morphometrics has the additional advantage of
62 a graphical means of displaying the nature of the shape differences between specimens or taxa using

63 thin plate spline deformations. However, in those cases where physical variables and/or landmarks
64 cannot be measured or determined across the whole spectrum of organisms that are being compared
65 (e.g., due to great variability, highly divergent body plans, or ambiguous primary homologies of the
66 landmarks), or where the variation among the organisms of interests transcends differences in shape
67 and includes other types of anatomical features, character-based analyses disparity are appropriate
68 [32,34-38,40,46]. Of course, such analyses are also suitable in those cases in which organisms are
69 directly comparable and statements of homology are clear, as in the anomodont example that is the
70 basis of the present study.

71 Character-based analyses of disparity rely on multivariate treatments of differences among
72 discrete and/or continuous traits, and these are codified in the form of states in phylogenetic data
73 matrices. The matrices may additionally encompass phenetic, ecological, environmental, and/or
74 functional data. When applied to morphological characters in a cladistic or phenetic framework, this
75 category of disparity methods provides a less intuitive treatment of morphological variation than
76 those offered by traditional or geometric morphometric methods. This is because the dissimilarity
77 among taxa is not measured using descriptors of physical shape (e.g., lengths, widths, angles, ratios,
78 positions of landmarks), but is instead quantified in terms of the amount of character-state or trait
79 variation that exists [32,40]. Therefore, the differences among taxa cannot be easily mapped back
80 on to the organisms as can be done for variations in linear dimensions or changes in overall shape.
81 Instead, they represent a summary of differences and these could take a variety of forms, ranging
82 from the presence or absence of, say, certain bones or organs, details of the contacts among bones,
83 features of the construction of complex structures, or the shape differences of those structures.

84 The characters used to build a phylogeny or a dendrogram can also be employed to construct
85 a multidimensional morphospace in which the distances between taxa reflect the magnitude of their
86 morphological differences. Again, it is important to remember that these distances are based on the
87 number of differences in the codings of characters that can cover a range of anatomical structures.
88 A given taxon may be located one unit away from a second taxon on account of the absence of a

89 bone, whereas it may be located one unit away from a third taxon on account of the combination of
90 bones that form its secondary palate. Therefore, although the distances among taxa in a character-
91 based morphospace reflect the fact that the taxa differ in a given number of character and/or trait
92 conditions, their positions in morphospace do not provide any direct and explicit information about
93 which characters differ between them.

94 Character-based analyses of disparity are not intrinsically superior/inferior to, nor are they a
95 substitute for, traditional or geometric morphometric studies; they are merely different. By focusing
96 on the number of differences among taxa, they can accommodate a greater variety of morphological
97 descriptors - cladistic, phenetic, functional, ecological, or otherwise [32,40,46] - in a simultaneous
98 analysis. They can further accommodate taxa that encompass widely divergent body plans and few
99 homologous landmarks. This flexibility comes at the cost of the difficulty of relating the distances
100 among taxa in morphospace to specific anatomical and/or shape differences, thus limiting to some
101 extent the insight they provide into topics such as convergent evolution. Character-based analyses
102 of disparity have been extensively used with cladistic data matrices of discrete traits (or, at least,
103 matrices that include a large proportion of such traits), but their utility is by no means restricted to
104 alphanumeric data sets. In fact, the data sets can accommodate a mixture of traits, e.g., discrete
105 (binary and/or multistate) and continuous, as well as different options for ordering and weighting.
106 Many such options are implemented in the versatile free software MATRIX v. 1.0 [32,38-45,47].

107

108 **(d) *Pair-wise taxon distances***

109 We built a tabulation of inter-taxon generalized Euclidean distances (Dataset S1) in MATRIX v. 1.0,
110 treating all characters as unordered and having equal unit weight, but without replacing instances of
111 polymorphic codings with known states (i.e., polymorphisms were treated as such). This practice
112 contrasts with those in other studies [40], where uncertain and polymorphic codings were replaced
113 with one of the alternative states that are bracketed under uncertainty or polymorphism (e.g., using
114 consistently the lowest or the highest of the bracketed states in each case). Our solution is thus more

115 conservative than that of previous analyses, though in many of the case studies published thus far,
116 the main results from disparity and morphospace analyses are not altered to a significant degree
117 when alternative codings are introduced as a replacement for uncertainties and polymorphisms. For
118 the 143 discrete characters, there are 22 instances of polymorphic codings (there are no uncertainties
119 in the data matrix), representing 0.177% of the total number of cell entries (12,441) for the discrete
120 characters.

121 When missing entries (i.e., unknown, inapplicable states, as well as question marks replacing
122 uncertainties or polymorphisms) occur in a pair-wise comparison between any two taxa, MATRIX
123 assigns a mean weighted value to the character comparisons for which one or both taxa exhibit the
124 missing entries. It first calculates a weighted mean fractional similarity (WMFS), namely the ratio
125 between the total distance for all the scorable comparisons between any two taxa (i.e., the number of
126 instances of observed mismatches in the known scores assigned to those taxa) and the total potential
127 distance for all the scorable comparisons (i.e., the maximum possible number of mismatches in the
128 actual compared scores, if these were to differ entirely in the two taxa in question). Second, each
129 instance of a character comparison for which one or both taxa show missing entries is replaced with
130 a value given by multiplying the WMFS by the potential distance. Third, the value thus obtained is
131 added to the distance obtained for the scorable comparisons, in order to give a corrected Manhattan
132 distance. Fourth, all the character distances are squared and summed. Fifth, the resulting values are
133 rooted to yield a generalized Euclidean distance between the two taxa in question [32].

134 In theory, different types of taxon-taxon distances could be used. We opted for the generalized
135 Euclidean distances because ordination methods (e.g., Principal Coordinates Analysis [32,38,40]; but
136 see also [46]) conducted on square dissimilarity matrices of Euclidean distances result in many fewer
137 ‘negative’ multivariate axes (which are difficult to interpret) than in the case of square dissimilarity
138 matrices consisting of, say, Manhattan distances. More fundamentally, the Euclidean nature of the
139 distance matrix is a logical prerequisite for geometric interpretations of patterns of morphospace
140 occupation (triangle inequality criterion holding strictly in a multidimensional Euclidean space). In

141 addition, although correction for negative axes is strictly speaking unnecessary with Euclidean
142 distances, we found that in practice, a variable number of such axes may still result from matrix
143 ordination. We therefore followed the practice of several recent works [38-45] in performing the
144 multivariate analysis of tabulated distances with negative eigenvalue correction.

145 Because the data matrix in [11] includes discrete binary, discrete multistate, and continuous
146 characters, we selected appropriate 'codes' in MATRIX for each character. Thus, code 'b' (for
147 binary) is appropriate when one wishes to record shared derived similarity (for instance, shared loss
148 of a feature; with this code, matches of '1's in two taxa yield a distance of '0', but other state-to-state
149 comparisons and matches of '0's yield a distance of '1'). Code 'm' (for multistate) is suitable for
150 multistate unordered discrete characters (identical states give a distance of '0'; different states give a
151 distance of '1'). Finally, we applied code 'r' (for ranged) to continuous characters (this code is also
152 suitable for multistate ordered discrete data), whereby the distance between two taxa is a fraction of
153 the range between the highest and lowest values in the set of continuous measurements [32,63].

154

155 **(e) *Multivariate analyses of pair-wise distances***

156 We applied Principal Coordinates (PCo) Analysis to the pair-wise generalized Euclidean distances
157 using GINKGO v. 1.5.5 [64], a free multi-platform Java application for multivariate analyses and
158 statistics (<http://biodiver.bio.ub.es/ginkgo/Ginkgo.htm>). We performed the PCo analysis with the
159 Cailliez method [65] of negative eigenvalue correction [66], placing the centroid for the 87 taxa on
160 the origin of the multivariate axes. PCo scores (i.e., PCo coordinates) for all taxa along each PCo
161 axis are tabulated in Dataset S2. We determined the number of ordination axes (PCo components)
162 to be retained for further analyses and tests by inspecting a semi-logarithmic scree plot in GINKGO
163 [67]. In this plot, the \log_{10} -transformed eigenvalues (representing the amounts of variance explained
164 by the principal coordinates) were plotted against axis number. The occurrence of a 'break' in the
165 distribution of log-transformed eigenvalues between PCo axes 9 and 10 (after which point no major
166 discontinuities could be observed) marked the threshold point for retaining 10 axes. Although other

167 criteria for axis retention are available, they provided less consistently meaningful results. As an
168 example, we could have used the number of axes that, together, summarize a given percentage of
169 the total variance in the data (e.g., 90%). However, it became apparent that many of the higher axes
170 differed little from one another and contributed little structure to the morphospace. The use of the
171 broken-stick method in the ‘ape’ library for ‘R’ (<http://www.r-project.org/>; [68]) also proved to be
172 unsatisfactory. Without negative eigenvalue correction, this method selected axis PCo1 only. With
173 negative eigenvalue correction, it selected axes PCo1-3. However, as explained above, higher axes
174 PCo4-10 still contribute to morphospace structure.

175

176 **(f) *Disparity metrics***

177 We used the PCo scores on the first 10 PCo axes to calculate four disparity metrics, namely the sum
178 and root-product of both ranges and variances. To this end, we used the RARE v. 1.2 disparity and
179 rarefaction software [32,38-45,47,63]. We show exclusively the results based upon the two sums, as
180 the root-products reveal very similar patterns. In a geometrically intuitive way, the sum of ranges
181 measures the amount of morphospace occupation, whereas the sum of variances measures the
182 spread of taxa relative to their own centroid (i.e., their mean configuration) [63]. For each disparity
183 metric, we built a complete rarefaction profile of mean and median values by extracting numerous
184 times (1000 bootstrap replicates) all the subsamples of taxa between 1 and the maximum number of
185 taxa in any specific set, such as a clade or a time interval (Datasets S3 and S4). We calculated 95%
186 confidence intervals for each subsampling routine. For disparity plots, we show both the un-rarefied
187 median value with the associated confidence interval for each disparity metric (using the maximum
188 number of taxa occurring in any specific taxon set), and the values generated by rarefaction of all
189 samples to the smallest taxon set (in order to standardize calculations by taking into account the
190 unevenness of sample sizes, i.e. taxon numbers, in the different sets).

191

192 **(g) *Morphospace plots***

193 Two- and three-dimensional plots using combinations of the first three PCo axes were inspected in
194 PAST v. 2.14 (<http://folk.uio.no/ohammer/past> [50]). To evaluate differences among groups, we
195 used a one-way analysis of similarities (ANOSIM: null hypothesis: equal median and range for
196 ranked dissimilarities within groups of interest; [69]) and a one-way non-parametric multivariate
197 analysis of variance (npMANOVA: null hypothesis: similar variances for groups of interest; [70]).
198 As non-parametric tests, ANOSIM and npMANOVA are useful in the absence of any information
199 on the distribution of scores on the PCo axes [40,41,50]. The results of both tests are reported in
200 Dataset S5.

201

202 **(h) *Experiments with autapomorphies***

203 The effects of autapomorphies on analyses of disparity and morphospace occupation require full
204 scrutiny. This issue was discussed briefly in [32,40,41], and has been raised more recently [46].
205 Although we reserve a more exhaustive treatment for a separate publication, some observations are
206 necessary before we describe our simulation experiments. These experiments provide empirical
207 evidence, based on the anomodont case study, that autapomorphies may not affect relative measures
208 of disparity (i.e., the profiles of increasing or decreasing disparity between groups) and patterns of
209 morphospace occupation to any significant extent.

210 There are practical limits to the way in which unique traits can be codified for any organisms.
211 Even within a specific morphofunctional complex, e.g. the skeletal system, autapomorphy selection
212 may be problematic for several reasons. First, the status of each character changes depending on the
213 level of phylogenetic and taxonomic inclusiveness, the practice of lumping or splitting species, and
214 different coding and ordering régimes. Second, the distinctiveness of taxa may rest either on truly
215 unique traits or on exclusive combinations of features that may be present in other taxa, including
216 plesiomorphies. However, recognition of genuinely unique features is hampered by subjective
217 evaluations of the comparative data at hand, character-state delimitations, failure to account for
218 variability, incompleteness of material, limited character atomization, and newly discovered taxa,

219 among other factors. Third, unless one or more taxa represent true outliers (e.g., due to their
220 extreme morphologies), the distribution of unique features among taxa under study might approach
221 randomness, and thus have little impact on relative disparity values (of course, absolute values will
222 change with autapomorphy inclusion) and on patterns of morphospace occupation (within- and
223 between-group distances will vary isometrically, or nearly so). However, even with outliers, it may
224 be possible to atomize characters in such a way that, for a seemingly unique feature X in taxon A,
225 there might be a unique feature Y in taxon B, a unique feature Z in taxon C, ..., etc. Furthermore,
226 the unique features X, Y, Z need not relate to the same structure. As a hypothetical example, we
227 might find unique and very subtle differences in ten femora belonging to ten anomodont species,
228 such that each has a distinctive trait of its own. For any given unique trait in the femur of an
229 anomodont species, there might be a unique trait of the cervical vertebrae in another species, and a
230 unique trait of the palate in yet another species. Ultimately, this atomization of traits will lead to
231 uniform distribution of autapomorphies across the data matrix. We seek to understand how realistic
232 this scenario is, and we want to determine how a non-random distribution of autapomorphies might
233 affect either disparity analyses or patterns of morphospace occupation.

234 To examine these issues, we performed a set of experiments designed to simulate occurrences
235 of various proportions of hypothetical unique features distributed in different ways among the 87
236 taxa. Starting with the original matrix of 163 characters [11], we built seven simulated data sets
237 consisting of hypothetical autapomorphies only, and added these to the existing character set. We
238 assumed that the hypothetical autapomorphies were discrete traits that could be coded in all taxa
239 (i.e., there were no instances of unknown conditions), such that in each case 86 taxa would be coded
240 as '0' and a single taxon would be coded as a '1'. Simulated sets were as follows:

241

242 a) Simulation 1: 250 characters (163 original, 87 hypothetical autapomorphies; 1 autapomorphy per
243 taxon).

244 b) Simulation 2: 424 characters (163 original, 261 hypothetical autapomorphies; 3 autapomorphies
245 per taxon).

246 c) Simulation 3: 598 characters (163 original, 435 hypothetical autapomorphies; 5 autapomorphies
247 per taxon).

248 d) Simulation 4: 1033 characters (163 original, 870 hypothetical autapomorphies; 10
249 autapomorphies per taxon).

250 e) Simulation 5: 580 characters (163 original, 417 hypothetical autapomorphies; average of 4.79
251 autapomorphies per taxon). In this experiment, each taxon was randomly given a number of
252 autapomorphies ranging between 1 and 10.

253 f) Simulation 6: 667 characters (163 original, 504 hypothetical autapomorphies; average of 5.79
254 autapomorphies per taxon). In this experiment, each Permian taxon was randomly given a number
255 of autapomorphies ranging from 5 to 10, and each Triassic taxon a number of autapomorphies
256 ranging from 1 to 5.

257 g) Simulation 7: 541 characters (163 original, 378 hypothetical autapomorphies; average of 4.34
258 autapomorphies per taxon). In this experiment, each Permian taxon was randomly given a number
259 of autapomorphies ranging from 1 to 5, and each Triassic taxon a number of autapomorphies
260 ranging from 5 to 10.

261

262 The logic behind these experiments is that in simulations 1-4, autapomorphies are distributed
263 uniformly among taxa, and their numbers per taxon increase regularly. Obviously one could create
264 infinite data sets with increasing numbers of unique traits added equally to all taxa. However, this
265 would result in little more than an isometric expansion of morphospace occupancy. Simulation 5 is
266 probably the most realistic, because autapomorphies are distributed at random among taxa. Finally,
267 the last two data sets (simulations 6 and 7) are designed to address the issue of uneven distributions
268 of unique traits in taxon partitions. Note that in the last two simulated data sets, the difference in

269 autapomorphies is consistent for all Triassic taxa (i.e., the two Triassic emydopoids, the species of
270 *Lystrosaurus* that have Triassic first appearances, and the kannemeyeriiforms).

271 Another way in which uneven distributions of autapomorphies could occur is by taxonomic
272 groups (clades or otherwise). However, devising simulations that accommodate this scenario would
273 entail a large number of possibilities. Furthermore, these simulations may be unwarranted for two
274 related reasons. First, we would have to postulate that the taxa in a given clade display an unusually
275 large number of traits not present in any other group. These traits would be autapomorphies for the
276 clade as a whole, and thus synapomorphies for its constituent taxa. In this respect, they would be
277 coded precisely as such - hypotheses of primary homology that have passed a congruence test
278 [71,72]. Second, even if these traits were distributed in some of the taxa only, or could not pass a
279 congruence test (thus appearing as homoplasies), they would still be coded as primary homologies
280 and incorporated into the data matrix in that way.

281 For each of the simulated data sets described above, we created a tabulation of generalized
282 Euclidean distances in MATRIX and subjected them to PCoA using GINKGO (Dataset S1).
283 Subsequently, we carried out a global Mantel test [73] using the free software CADM [74], also
284 implemented in the 'ape' library for 'R' (<http://www.bio.umontreal.ca/casgrain/en/labo/cadm.html>).
285 CADM first outputs results for the global test of overall incongruence among distance matrices
286 (null hypothesis: incongruence of all matrices; statistics: Kendall's W coefficient of concordance
287 and Friedman's X^2 for permutational tests of W). The matrices are subsequently permuted at
288 random and independently, and a second test is provided for the null hypothesis that each matrix is
289 incongruent with each of the other matrices in turn (statistics: rank-based [Spearman] Mantel
290 correlations, and associated permutational probability). In addition, we conducted a posteriori
291 permutation tests of the contributions of each distance matrix from a particular simulation to the
292 overall concordance among the matrices. Tests were performed with 999 random permutations of
293 matrix structure, and each matrix was given equal weight. In addition, for a posteriori permutation

294 tests we applied the Holm-Bonferroni correction of p values for multiple pair-wise comparisons
295 (Dataset S7).

296

297 **(i) *Taxon partitions by groups***

298 We performed a series of experiments using different types of taxon and character partitions. Taxon
299 partitions for disparity analyses through time (Dataset S3) and by major groups (Dataset S4) were
300 detailed in the main text.

301 As a frame of reference for the study of disparity changes across the evolutionary history of
302 anomodonts, we used the tree topology in figure S1 in order to delimit nine groups. Five of these
303 groups are paraphyletic assemblages (grades), whereas the remaining four are monophyla (clades).
304 There are various ways in which we could delimit groups. Our preferred solution gives a trade-off
305 between reflecting the sequence of key branching events in anomodont evolution and including the
306 several newly recognized levels of morphological organization in the clade as a whole [11]. The
307 nine major groups (and associate colour-codings) are: g1 = basal anomodonts, dark gray; g2 =
308 endothiodonts, dark magenta; g3 = emydopoids, cyan; g4 = cryptodonts, green; g5 = ‘*Dicynodon*’-
309 grade taxa, brown; g6 = lystrosaurids, red; g7 = dinodontosaurids plus shansiodontids, lime; g8,
310 kannemeyeriids, light blue; g9 = stahleckeriids, dark blue.

311

312 **(j) *Taxon partitions by time intervals***

313 We considered two sets of chronological taxon partitions. The first partition consisted of Permian
314 (P) and Triassic (T) intervals. The second partition consisted of stage-level intervals, as detailed in
315 the main text. The merging of some stages into longer time intervals was dictated by the paucity
316 (Roadian; Norian) or absence (Olenekian) of taxa in some stages. Stage-level time intervals are as
317 follows: t1 = Roadian-Wordian; t2 = Capitanian; t3 = Wuchiapingian; t4 = Changhsingian; t5 =
318 Induan-Olenekian; t6 = Anisian; t7 = Ladinian; t8 = Carnian-Norian.

319

320 **(k) *Character partitions: cranial vs. postcranial and discrete vs. continuous***

321 In order to evaluate the extent to which different skeletal regions and different types of characters
322 may affect patterns of morphospace occupancy, we partitioned the data matrix in [11] into cranial vs.
323 postcranial characters, as well as into discrete vs. continuous characters. For each character partition,
324 we performed Mantel tests to assess the correlation between the two sets of pair-wise taxon distances
325 derived from the partitions of interest (e.g., cranial vs. postcranial; discrete vs. continuous) (Dataset
326 S7). For the cranial vs. postcranial data partition, it was necessary to prune the original data matrix,
327 so as to produce the largest possible set of taxa for which the two character subsets could be coded
328 (i.e., we deleted all taxa that were entirely scored as unknown in either the cranial or the postcranial
329 data). This resulted in 54 taxa being retained. No taxon deletion was necessary for the partition into
330 discrete vs. continuous characters.

331

332 **SUPPLEMENTARY RESULTS**

333 **(a) *Results of Principal Coordinates Analysis***

334 PCoA of the pair-wise taxon distances built from the data matrix in [29] results in the first 10 PCo
335 axes explaining 24.512% of the total variance. PCo axes 1-3, used to show patterns of distribution
336 of taxa in morphospace, summarize 6.643%, 3.0989%, and 2.4111% of total variance, respectively.

337

338 **(b) *Distribution of anomodonts in morphospace***

339 The two-dimensional morphospace plots delimited by combinations of the first three PCo axes
340 (figure 1a, b) show the following main features. First, basal anomodonts (g1) occupy a much larger
341 region of morphospace than all other groups (g2-g9) and despite their low taxic diversity, they are
342 highly dispersed around their own centroids. Second, endothiodonts and emydopoids (g2 and g3)
343 overlap considerably in morphospace, but tend to remain separate from more apical groups (g4-g9).
344 Among the latter groups, consistent and conspicuous overlap characterizes *Dicynodon*-grade taxa
345 (g5) and lystrosaurids (g6), on the one hand, and kannemeyeriids (g8) and stahleckeriids (g9), on the

346 other. Third, increasingly apical groups - especially g8 and g9 - form progressively more compact
347 clusters in morphospace (though g4 - the cryptodonts - is an exception).

348 The ANOSIM and npMANOVA tests corroborate in part the patterns expounded above. Both
349 ANOSIM ($R = 0.6531$; $p = 0.0001$) and npMANOVA ($F = 13.5$; $p = 0.0001$) results reject the null
350 hypothesis of no differences in morphospace distribution among the nine major groups. In both tests,
351 two post-hoc pair-wise comparisons are not significant, specifically those between g2 and g3 and
352 between g8 and g9. Furthermore, in the case of ANOSIM an additional non-significant comparison
353 is between g1 and g2.

354 When we introduce autapomorphies according to the simulations 1-7 described above, a global
355 Mantel test indicates a strong and significant overall positive correlation for the ensemble of the
356 generalized Euclidean distances based on the original data matrix and the distances obtained from
357 each of the simulations ($W = 0.90671$; $X^2 = 27128.76226$; $p = 0.001$). Correlations in each pair-wise
358 comparison of distance sets generated from simulations tend to be higher than the correlations
359 between the original distances and the distances from each simulation. This result suggests that,
360 regardless of number and distribution of autapomorphies, they have little impact on the relationships
361 among intertaxon distances. However, correlation values are moderate to high even in the case of
362 original and simulated distances. The lowest value is for distances from simulation 6, where we
363 assigned at random a number of autapomorphies ranging from 5 to 10 to Permian taxa, and from 1 to
364 5 to Triassic taxa. The highest value is for distances from simulation 1 - perhaps unsurprisingly, as
365 this simulation implies addition of just one unique trait to each taxon - followed by the values for
366 simulations 4 (second highest) and 2 (third highest). The four lower values, for simulations 3, 5-7,
367 are nevertheless still substantial and of those, the value for simulation 5 is the highest (this is the
368 most realistic experiment, implying addition of autapomorphies at random across the matrix).

369 For each simulation, two-dimensional scatter biplots delimited by the first two PCo axes
370 (easily derived using Dataset S2) show that (1) placements of groups g1-g9 relative to each other
371 are only slightly altered by the inclusion of autapomorphies, (2) most of the individual taxa occur in

372 similar relative positions, and (3) the relative sizes of the groups in morphospace are affected to a
373 negligible degree. The plot from simulation 4 may appear at odds with all the others; however, this
374 is due to the fact that it is actually merely reflected along PCo axis 2, so that the basic relationships
375 and arrangement of taxa are still essentially the same. The most conspicuous change relative to the
376 plot from the original matrix is that adding autapomorphies tends to “smear” groups out over larger
377 areas of morphospace (most convex hulls delimiting groups appear to be “stretched”). This change
378 appears to be quite consistent, even when the number of autapomorphies per taxon is introduced at
379 random (e.g., as in simulation 5). These observations also hold true for simulations 6 and 7, where
380 autapomorphies have different frequencies among Permian and Triassic taxa.

381

382 ***(c) Effects of character partitions***

383 Despite the reduced number of taxa in the comparison between morphospace plots generated from
384 cranial and postcranial data, we found that pair-wise distances derived from cranial data correlate
385 significantly, albeit only moderately, with those derived from postcranial data (Dataset S7). Since
386 discrete characters constitute the greatest proportion of all characters in the original matrix [11], we
387 expect the mutual positions of taxa in the discrete trait-based morphospace to be similar to the plot
388 generated using all characters. This is indeed the case: groups g1-g9 show nearly identical relative
389 arrangements and patterns of overlap to those in figure 1. When only continuous data are employed,
390 however, substantial changes characterize the distribution of taxa. Thus, the nine major groups tend
391 to overlap more extensively. Furthermore, except for a small number of outliers in groups 1 and 9,
392 most remaining taxa form a compact cluster. These results are hardly surprising, given the highly
393 divergent cladogram obtained from running a phylogenetic analysis employing only the continuous
394 characters [11]. Results from the Mantel test show that the correlation between the distances from
395 discrete characters and those from continuous characters are invariably very low for all correlation
396 coefficients (though such coefficients differ significantly from random).

397

398 **(d) *Patterns of morphological disparity***

399 In the following, it is useful to report modalities of overlap among confidence intervals as a way to
400 assess significant (non-overlap) or non-significant (overlap) differences between adjacent disparity
401 values [30]. Invariably, both disparity metrics (sums of ranges and variances) show Permian taxa to
402 be significantly more disparate than Triassic taxa, regardless of whether rarefaction is used (figure
403 S2a, b). Temporal disparity profiles are more patterned when analyzed by stage subdivisions (figure
404 S2c, d).

405 Plots using the rarefied sums of ranges and variances and the un-rarefied sum of variances are
406 similar to one another and indicate a general, steady decrease in median disparity values from
407 Roadian-Wordian (t1) (or Capitanian, t2, in the case of the rarefied sum of ranges) through to t8
408 (Carnian-Norian). In those three plots, disparity values in time bins t1-t4 (or t2-t4) appear to be
409 significantly different from those in time bins t7 and t8. Again in the same plots, disparity in the
410 Induan-Olenekian (t5) is not significantly different from disparity in all (or most, in the case of the
411 un-rarefied sum of variances) other stages. The plot for the un-rarefied sum of ranges is utterly
412 discordant from the other three plots examined so far. In particular, median values of disparity
413 increase steeply from t1 to t2, fluctuate to a negligible extent in time bins t2-t4 (characterized by a
414 small decrease), then drop dramatically across the PTB. During the Triassic, anomodont disparity
415 experienced a new slight increase during t6, reaching a level comparable to that in t1. Finally, we
416 observe a new steady decrease from t6 to t8.

417 Finally, we consider the contributions of individual groups to overall disparity (figure S2e, f).
418 There are striking similarities in the profiles of disparity values from g1 through to g9 when either
419 the sum of ranges or the sum of variances is used as metric. Furthermore, the un-rarefied and rarefied
420 profiles also differ little from one another. The subtle differences between un-rarefied and rarefied
421 plots, and between the two disparity metrics, are best captured in visual inspections of the plots. We
422 therefore focus mostly on common patterns gleaned from each disparity plot.

423 In all plots, basal anomodonts (g1) and cryptodonts (g4) exhibit, respectively, the highest and
424 lowest median disparity values. In addition, the confidence interval for g1 shows very small or no
425 overlap with the confidence intervals for other groups, indicating significant or nearly significant
426 differences from those. Somewhat intermediate between g1 and g4 - though closer to g4 than to g1 -
427 are the comparable disparity values for endothiodonts (g3) and emydopoids (g4). Across groups g5
428 through to g9, the general trend is one of slow and negligible decrease in disparity, particularly
429 evident in g6 (lystrosaurids), g7 (dinodontosaurids plus shansiodontids), and g8 (kannemeyeriids).
430 In addition, confidence intervals for these five groups tend to overlap extensively, indicating no
431 significant differences in disparity values among them.

432

433 **(e) *Decoupled disparity and diversity***

434 The plots in figures 3, S3, and S4 illustrate trends in disparity and diversity. These use all possible
435 combinations of disparity metric (sum of ranges; sum of variances), correction for sample size (un-
436 rarefied; rarefied), time series co-variation (raw data in time bins; generalized differencing of time
437 series), taxic diversity (number of taxa used in cladogram; total number of anomodont taxa recorded
438 so far; total number of major anomodont lineages). The non-significant correlation between the two
439 sets of values (diversity; disparity) is borne out by the vast majority of calculations. However, there
440 are three instances of significant comparisons. All involve generalized differencing treatment for the
441 sum of ranges and generalized differencing for one of the following variables: number of taxa per
442 time interval actually present in the phylogeny; total number of known anomodont taxa recorded in
443 each time interval; and number of major lineages per time interval.

444 Taxic diversity is often decoupled from morphological disparity [75-77], and both variables
445 may be affected by the use of different taxonomic ranks and preservation biases. It is commonly
446 assumed that survivors of major extinction events undergo relatively rapid morphological
447 diversification into supposedly empty ecospace. A clear understanding of these patterns in terrestrial

448 vertebrates requires study of diversity, ecological shifts, and morphofunctional change through the
449 time intervals of recovery [78-87].

450 There are potential issues with the quality of data in considering any aspect of the fossil record
451 [88-90]. A number of authors [89] have argued that the terrestrial record is especially incomplete,
452 and several have employed uncorrected data sets in macroevolutionary studies. However, for some
453 vertebrate clades the available paleontological documentation has been shown to be adequate [90],
454 and we reserve a detailed analysis of the impact of geological biases on anomodont diversity and
455 disparity through time for a separate publication. For the purposes of the present study, we note that
456 the sample of taxa is an adequate representation of known anomodont diversity at genus and, to a
457 more limited extent, species levels. As we employ different disparity metrics (each of which is
458 sensitive to various parameters), we can correct for possible biases introduced either by taxon sample
459 size (e.g., occurrence of outliers) or by taxonomic practice (e.g., by considering genera rather than
460 species, therefore avoiding the issue of taxonomic splitting/lumping).

461 At a more general level, note that local-scale investigations of both South African and Russian
462 Permo-Triassic sequences [91-93] have demonstrated that intensity of sampling increases through
463 the Early Triassic, the very time when diversity and disparity are lowest for several groups of
464 organisms. In fact, it has recently been pointed out [91,92,94,95] that the earliest Triassic time
465 intervals represent distinct outliers with unusually low taxon counts despite increased sampling.
466 Hence, the paleontological record (at least in those two key cases) may contain more biological than
467 geological signal, as these low taxon counts certainly are the result of the end-Permian mass
468 extinction. Interestingly, different sampling proxies used in the same study area often reflect the
469 same pattern, suggesting that they are converging on approximately the same sampling signal.
470 Hence, it remains essential to explore the relationship between varying sampling proxies and
471 diversity in more detail across a wide range of clades. The presentation of both raw and corrected
472 diversity estimates [96,97] should be preferred to enable a comparison between both signals and to
473 identify similarities as well as potential differences and their consequences.

474

475 **SUPPLEMENTARY DATASETS**

476 **Dataset S1.** Tabulation of pair-wise generalized Euclidean distances for the original data matrix, for
477 each of the seven simulations with autapomorphy inclusions, and for each of the character partitions
478 (cranial; postcranial; discrete; continuous).

479 **Dataset S2.** Tabulation of Principal Coordinates scores derived from Principal Coordinates analyses
480 of the pair-wise generalized Euclidean distances for the original data matrix, for each of the seven
481 simulations with autapomorphy inclusions, and for each of the character partitions (cranial;
482 postcranial; discrete; continuous).

483 **Dataset S3.** Complete rarefaction profiles for sums and root-products of ranges and variances,
484 including mean, median, and upper and lower bounds of 90% confidence intervals, calculated for
485 eight stage-level time bins (t1 = Roadian-Wordian; t2 = Capitanian; t3 = Wuchiapingian; t4 =
486 Changhsingian; t5 = Induan-Olenekian; t6 = Anisian; t7 = Ladinian; t8 = Carnian-Norian) and two
487 system-level time bins (Permian; Triassic).

488 **Dataset S4.** Complete rarefaction profiles for sums and root-products of ranges and variances,
489 including mean, median, and upper and lower bounds of 90% confidence intervals, calculated for
490 nine major groups (g1 = basal anomodonts; g2 = endotheriodonts; g3 = emydopoids; g4 =
491 cryptodonts; g5 = 'Dicynodon'-grade taxa; g6 = lystrosaurids; g7 = dinodontosaurids plus
492 shansiodontids; g8, kannemeyeriids; g9 = stahleckeriids).

493 **Dataset S5.** Tests of the separation among the nine major anomodont groups in morphospace, using
494 Principal Coordinates on the first 10 axes, and Bonferroni correction of p values.

495 **Dataset S6.** Tests of the correlation between diversity and disparity through time, using un-rarefied
496 and rarefied sums of ranges and variances, total number of described anomodonts and number of
497 taxa in the phylogeny, and number of lineages. For all calculations, we also report results from
498 generalized differencing.

499 **Dataset S7.** Tests of correlations among distance matrices obtained from the original data matrix,
500 from each of the seven simulations with autapomorphy inclusions, and from each of the character
501 partitions (cranial; postcranial; discrete; continuous).

502

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726 **SUPPLEMENTARY FIGURES**

727 **Figure S1.** Anomodont phylogeny, based on analysis in [11].

728 **Figure S2.** Un-rarefied median disparity values and associated confidence intervals, based on the
729 sum of ranges (left column plots) and the sum of variances (right column plots); vertical grey bars
730 in (a-d) mark the Permian-Triassic boundary. (a-b) Disparity in Permian (P) and Triassic (T) taxa;

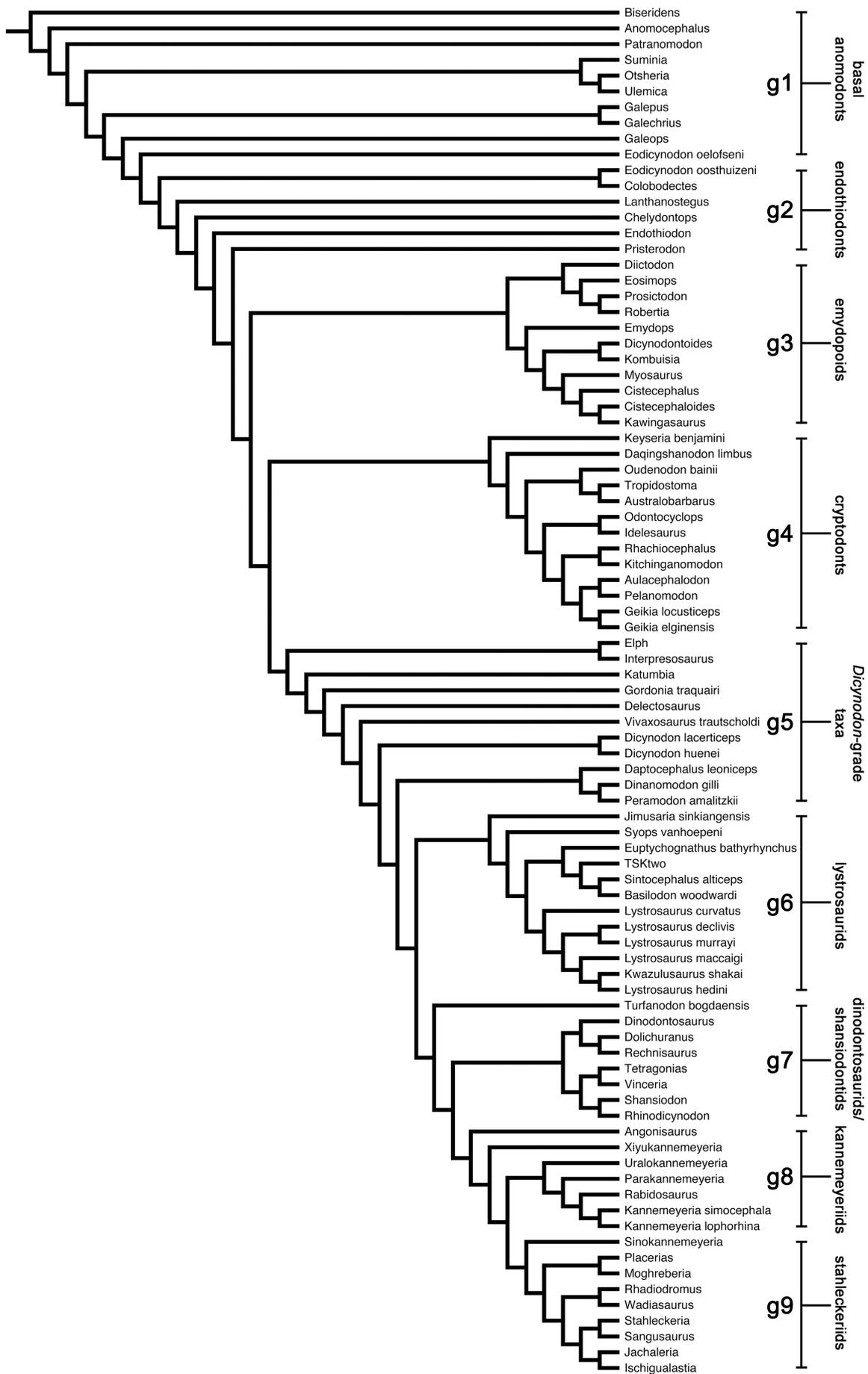
731 (*c-d*) disparity of taxa assigned to time intervals t1-t8 (see figure 2 for interval abbreviations); (*e-f*)
732 disparity of taxa assigned to groups g1-g9 (see figure 1 for group notations and color codes).

733 **Figure S3.** Comparisons between anomodont disparity (un-rarefied median values, grey circles)
734 and diversity (white squares) through time intervals t1-t8; disparity values are for the sum of ranges
735 (left column plots) and the sum of variances (right column plots); symmetric error bars around the
736 diversity values are calculated as $\pm\sqrt{N}$, where N is the number of taxa in a given time interval;
737 vertical grey bars mark the Permian-Triassic boundary. (*a-b*) Comparisons based on the number of
738 taxa actually present in the phylogeny; (*c-d*) comparisons based on the total number of known
739 anomodont taxa.

740 **Figure S4.** Comparisons between anomodont disparity (median values, grey circles) and diversity
741 (white squares) through time intervals t1-t8; disparity values are for the sum of ranges (left column
742 plots) and the sum of variances (right column plots); diversity is expressed as the number of major
743 lineages (groups g1-g9) present in a given time interval; vertical grey bars mark the Permian-
744 Triassic boundary. (*a-b*) Comparisons based on rarefied disparity values; (*c-d*) comparisons based
745 on un-rarefied disparity values.

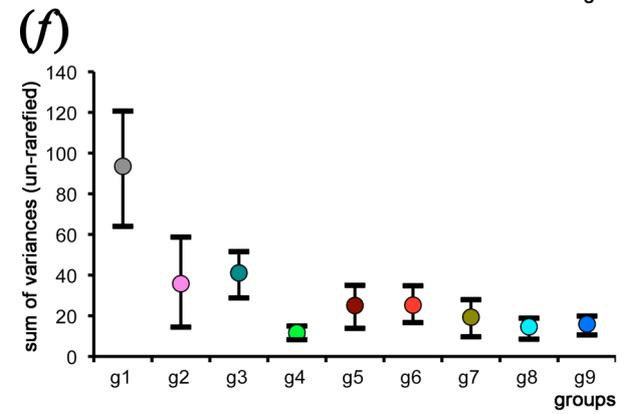
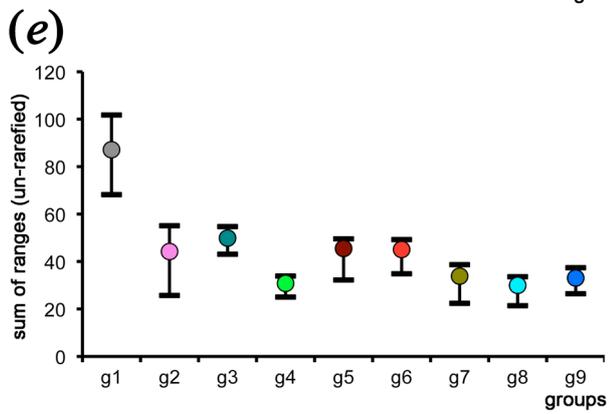
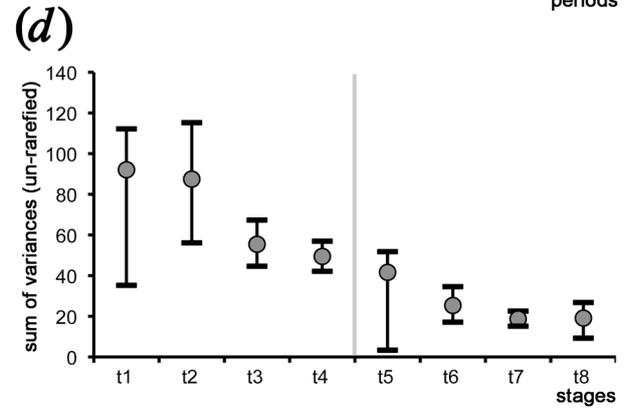
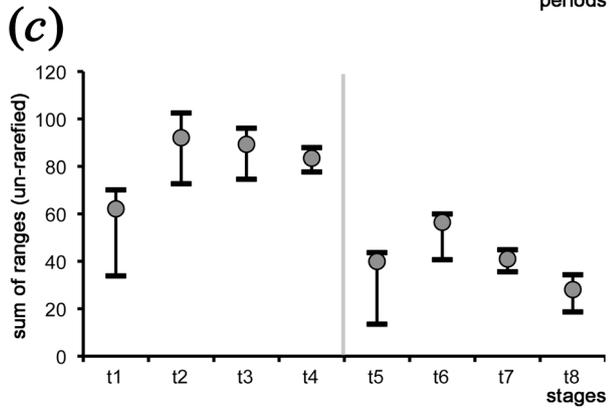
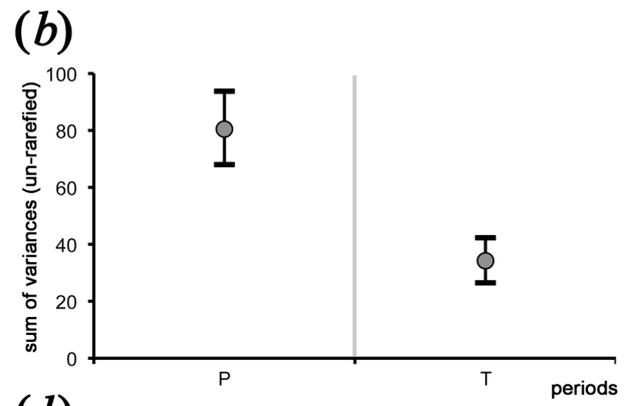
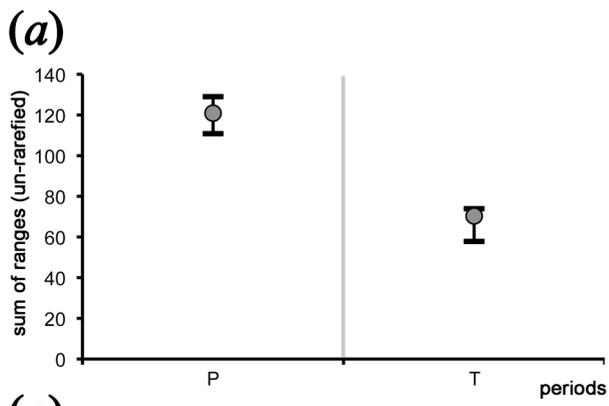
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748 **figure S1**



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750 **figure S2**

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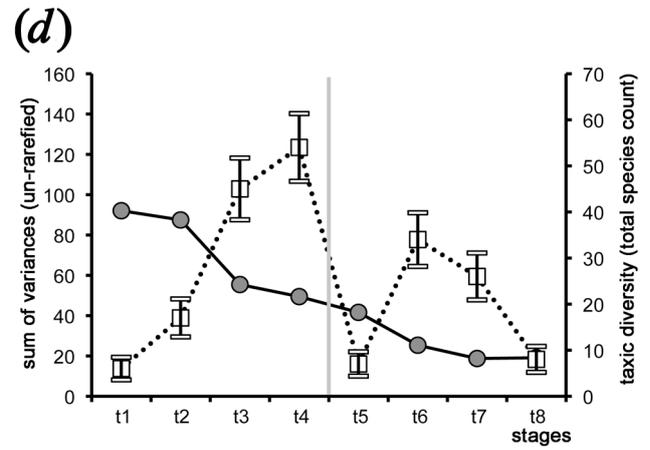
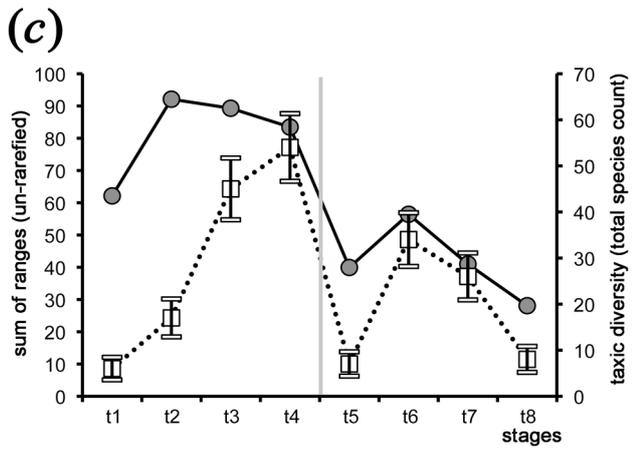
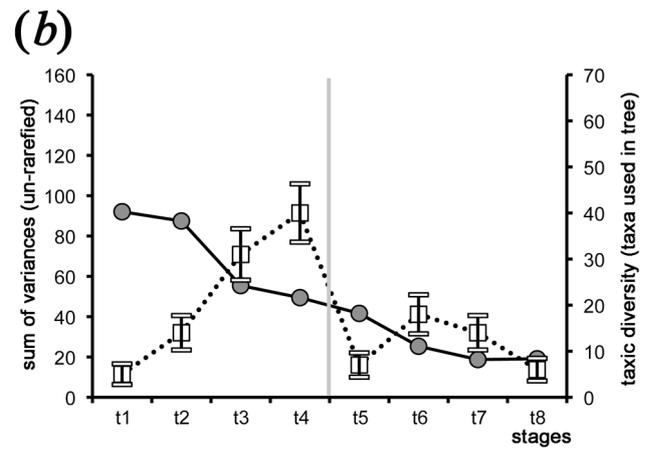
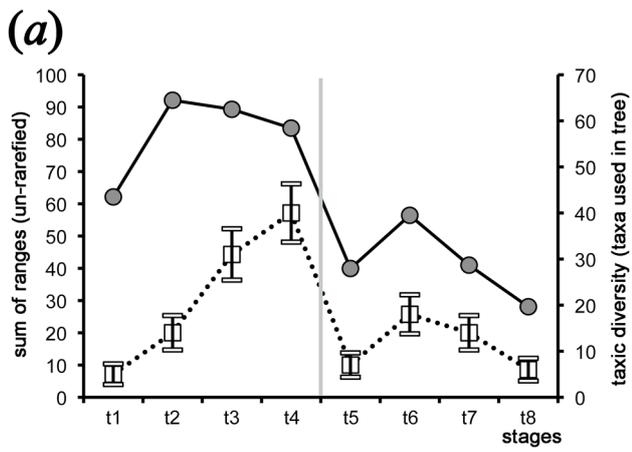
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760 **figure S3**

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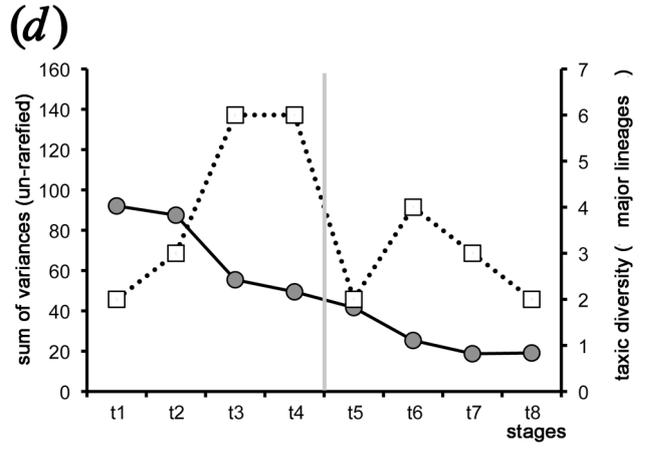
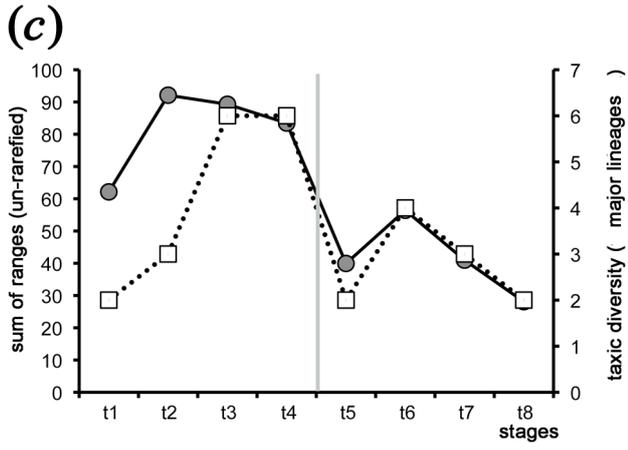
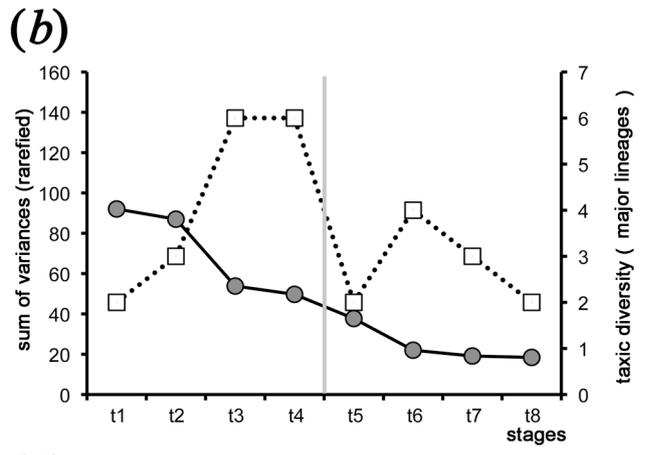
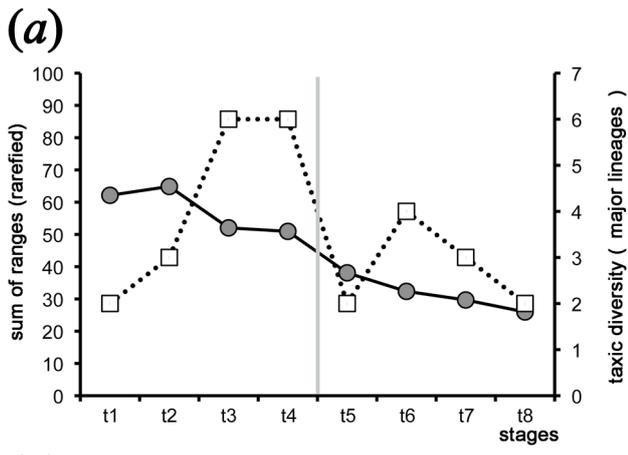
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775 **figure S4**