Morphospace saturation in the stem-gnathostomes *Pteraspidiformes heterostracans*: an early radiation of a 'bottom' heavy clade

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Ostracoderms (fossil armoured jawless fishes) shed light on early vertebrate evolution by revealing the step-wise acquisition of jawed vertebrate characters, and were important constituents of Middle Palaeozoic vertebrate faunas. A wide variety of head shield shapes are observed within and between the ostracoderm groups, but the timing of these diversifications and the consistency between different measures of their morphospace are unclear. Here, we present the first disparity (explored morphospace) versus diversity (number of taxa) analysis of Pteraspidiformes heterostracans using continuous and discrete characters. Patterns of taxic diversity and morphological disparity are in accordance: they both show a rise to a peak in the Lochkovian followed by a gradual decline in the Middle-Late Devonian. Patterns are largely consistent for disparity measures using sum of ranges or total variance, and when using continuous or discrete characters. Pteraspidiformes heterostracans can be classified as a "bottom-heavy clade", i.e. a group where a high initial disparity decreasing over time is detected. In fact, the group explored morphospace early in his evolutionary history, with much of the subsequent variation in dermal armour occurring as variation in the proportions of already evolved anatomical features. This early Early Devonian radiation is also in agreement with the paleobiogeographic distribution of the group, with a maximum of dispersal and explored morphospace during the Lochkovian and Pragian time bins.

Morphospace saturation in the stem-gnathostome~~s~~ ~~P~~teraspidiform~~es~~ heterostracans: an early radiation of a 'bottom' heavy clade

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ABSTRACT

Ostracoderms (fossil armoured jawless fishes) shed light on early vertebrate evolution by revealing the step-wise acquisition of jawed vertebrate characters, and were important constituents of Middle Palaeozoic vertebrate faunas. A wide variety of head shield shapes are observed within and between the ostracoderm groups, but the timing of these diversifications and the consistency between different measures of their morphospace are unclear. Here, we present the first disparity (explored morphospace) versus diversity (number of taxa) analysis of Pteraspidiformes heterostracans using continuous and discrete characters. Patterns of taxic diversity and morphological disparity are in accordance: they both show a rise to a peak in the Lochkovian followed by a gradual decline in the Middle-Late Devonian. Patterns are largely consistent for disparity measures using sum of ranges or total variance, and when using continuous or discrete characters. Pteraspidiformes heterostracans can be classified as a “bottom-heavy clade”, i.e. a group where a high initial disparity decreasing over time is detected. In fact, the group explored morphospace early in ~~his~~ evolutionary history, with much of the subsequent variation in dermal armour occurring as variation in the proportions of already evolved anatomical features. This early Early Devonian radiation is also in agreement with the paleobiogeographic distribution of the group, with a maximum of dispersal and explored morphospace during the Lochkovian and Pragian time bins.

INTRODUCTION

Ostracoderms (extinct, bony jawless vertebrates) are a paraphyletic assemblage comprising the jawed vertebrate stem group, which dominated the early vertebrate assemblages, first appearing with high levels of diversity in the Silurian (Sansom, Randle & Donoghue, 2015). Seen within the ostracoderms are many novel vertebrate features such as the first appearance of mineralised bone, paired appendages and paired sensory organs (Donoghue & Keating, 2014). The diversity of headshield shapes is large, with many groups variously possessing lateral, anterior and dorsal processes. The timing and nature of these morphological diversifications is unclear, as is the best way to quantify the morphological variation. For example, the difficulty in taxonomic assignment and phylogenetic reconstruction of the Pteraspidiformes (the largest clade of heterostracan ostracoderms) can be attributed to the continuous variation in their dermal plates which is often used to discriminate between taxonomic grades (Ilyes & Elliott, 1994; Pernègre, 2002; Pernègre & Goujet, 2007; Pernègre & Elliott, 2008; Randle & Sansom, 2017a; Randle & Sansom, 2017b). The Pteraspidiformes are characterised by possessing separate dorsal, ventral, rostral and pineal plates along with paired branchial, orbital and in some instances cornual plates (Fig. 1D)(Blieck, 1984; Blieck, Elliott & Gagnier, 1991; Janvier, 1996; Pernègre & Elliott, 2008; Randle & Sansom, 2017a; Randle & Sansom, 2017b). The Pteraspidiformes include many families and taxa of uncertain affinities. The Anchipteraspididae and *Protopteraspis* are stratigraphically the oldest Pteraspidiformes first occurring in the Pridoli (Elliott 1983; Blieck 1984; Blieck & Tarrant 2001). The Anchipteraspididae and *Protopteraspis* are both small Pteraspidiformes with blunt shaped ~~rostrums~~ (Fig. 1E). The Anchipteraspididae have a few anatomical differences to the remaining Pteraspidiformes including; a pineal plate enclosed within their dorsal plate, rather than positioned between the rostral and dorsal plates seen in all other Pteraspidiformes, a fused orbito-cornual plate (with are completely separate in other Pteraspidiformes taxa) and the centre of growth in the dorsal plate anterior to the midline, whereas, in other forms it is centrally or posteriorly positioned (Randle & Sansom 2017a; Elliott 1983). Other families include the Rhinopteraspididae (Fig. 1E), which contains taxa with extremely lengthened ~~rostrum~~ and headshields e.g. *Rhinopteraspis* and *Althaspis*, the Protaspididae, which contains taxa with widened headshields and forms with posteriorly extended branchial plates and absent cornual plates, and finally the Doryaspididae, containing the enigmatic *Doryaspis,* which has an unusually dorsally orientated mouth, extreme laterally extended cornual plates and unique pseudorostum (White 1935; Janvier 1996; Pernègre 2002). Randle & Sansom (2017a) also found the two Psammosteidae taxa to be nested within the Pteraspidiformes. The Psammosteidae are stratigraphically the youngest heterostracans and are characterised by having a dorsally orientated mouth and small ‘platelets’ separating their major plates (Blieck 1984; Janvier 1996)(Fig. 1E).

Due to the Pteraspidiformes possessing a rather uniform anatomy, inclusion of taxonomically informative quantitative data, including the relative sizes and dimensions of dermal plates, was explored in the phylogenetic analyses of Randle & Sansom (2017a), who included two different treatments of quantitative ratio data in their phylogenetic analyses of the Pteraspidiformes. The first treatment discretised the quantitative data into ordinal discrete character states by identifying gaps between the differences of ordered ratio data (>2 standard deviations of the gap data) to infer changes in character states. The second treatment used the raw continuous quantitative data to reconstruct their evolutionary relationships. Inclusion of quantitative data greatly improved the resolution of Pteraspidiformes relationships using traditional discrete characters – however, the two methods provided different and conflicting evolutionary relationships.

One of the goals of this study is to explore morphospace occupation through time using both classic discrete cladistic characters and quantitative continuous characters, along with the signal these phylogenetic morphospace plots provide for the different taxonomic clades within the Pteraspidiformes.

The use of cladistic or more traditional morphometric characters is debated in macro-evolution fields with authors arguing that discrete and morphometric characters differ in relative degree of independence, homology of the considered features, rate of evolution and ~~on~~ the nature of the variation being captured (MacLeod 2002; Klingenberg & Gidaszewski 2010). Mongiardino Koch *et al*. (2017) when exploring the scorpion genus *Brachistosternus*~~,~~ morphospaces derived from discrete and morphometric characters found the signal derived from these two different data types to be significantly different from each providing a non-congruent picture of their early evolution. For example, their discrete data displayed an ‘early burst’ scenario, whereas their morphological data did not, which they concluded was due to evolution being driven by species-specific adaptations of morphometric traits. On the contrary, several studies have shown empirically how the results derived from discrete and morphometric characters are fully compatible, providing the same signal on a macro-evolutionary scale (e.g. Villier & Eble, 2004; Anderson & Friedman, 2012; Foth et al., 2012; Hetherington et al., 2015;

Romano et al., 2017). It will be interesting to see if the two different data type i.e. discrete-with discretised and continuous characters display similar evolutionary scenarios. The specific clade of Pteraspidiformes therefore represents a new interesting case to empirically test the possible congruence between the signals contained in the discrete and morphometric characters.

Important in this context is whether timing of morphospace occupations as either early or late in the history of a clade and how they compare to changes in taxic diversity. Studies of morphospace occupation in both invertebrates (e.g. Foote, 1994, 1999; Lofgren, Plotnick, & Wagner, 2003; Villier & Eble, 2004; Lefebvre et al., 2006; Al-Sabouni, Kucera, & Schmidt, 2007; Scholz & Hartman, 2007; Glaubrecht, Brinkmann, & Pöppe, 2009; Whiteside & Ward, 2011; Deline & Ausich, 2011; Bapst et al., 2012; Hopkins, 2013; Romano et al., 2018) and vertebrates (e. g. Prentice, Ruta, & Benton, 2011; Benson, Evans, & Druckenmiller, 2012; Ruta et al., 2013; Colombo et al., 2015; Marx & Fordyce, 2015; Larson, Brown, & Evans, 2016; Romano, 2017; Romano et al., 2017) have reconstructed the timing of radiations, with many identifying maximum disparity at the beginning of their evolutionary history (termed ‘bottom heavy’), followed by stabilization and constant decrease until their subsequent extinction (e.g. Gould, Gilinsky, & German, 1987; Foote, 1992, 1994, 1995, 1999; McGhee, 1995; Wagner, 1995; Smith & Bunje, 1999; Eble, 2000; Huntley, Xiao, & Kowalewski, 2006; Ruta et al., 2013; Marx & Fordyce, 2015; Romano, 2017). Here we test the timing of morphospace radiations for Pteraspiformes and compare that to taxic diversity. We compare total variance or as a sum of ranges as measures of disparity, in both discrete and continuous sub-datasets.

MATERIAL AND METHODS

Taxa

The analysis was conducted using the phylogenetic analysis dataset of Pteraspidiformes heterostracans recently published by Randle & Sansom (2017a). For the study only the 49 in-group taxa of the original dataset were considered as follows: *Alaeckaspis*, *Althaspis*, *Anchipteraspis*, *Blieckaspis*, *Brachipteraspis*, *Canadapteraspis*, *Cosmaspis*, *Cyrtaspidichthys*, *Djurinaspis*, *Dnestraspis*, *Doryaspis*, *Drepanaspis*, *Errivaspis*, *Escharaspis*, *Eucyclaspis*, *Europrotaspis*, *Gigantaspis*, *Helaspis*, *Lamiaspis*, *Lampraspis*, *Larnovaspis*, *Loricopteraspis*, *Miltaspis*, *Mylopteraspis*, *Mylopteraspidella*, *Oreaspis*, *Palanasaspis*, *Panamintaspis*, *Parapteraspis*, *Pavloaspis*, *Pirumaspis*, *Podolaspis*, *Protaspis*, *Protopteraspis gosseleti*, *Protopteraspis primaeva*, *Psammosteus*, *Psephaspis*, *Pteraspis*, *Rachiaspis*, *Rhinopteraspis*, *Semipodolaspis*, *Stegobranchiaspis*, *Tuberculaspis*, *Ulutitaspis*, *Unarkaspis*, *Woodfjordaspis*, *Xylaspis*, *Zascinaspis carmani*, *Zascinaspis heintzi*. The taxa *Anglaspis*, *Athenaegis* and *Nahanniaspis* chosen as outgroups by Randle and Sansom (2017a) ~~differently~~ were not considered for the study of diversity and disparities through time. Thus, apart from the four species *Protopteraspis gosseleti*, *Protopteraspis primaeva*, *Zascinaspis carmani* and *Zascinaspis heintzi*, the ~~great part~~ of taxa are considered at the genus level. Foote (1995, 1996) has empirically shown how analysis conducted at the species and genus level provide equivalent signal (however Smith & Lieberman, 1999 consider the species level as preferable).

Diversity and disparity

To perform the analysis the following six time bins were selected spanning from the Upper Silurian to the Upper Devonian: Pridoli, Lochkovian, Pragian, Emsian, Eifelian, Givetian-

Frasnian. The Givetian and Frasnian stages were considered in a single time bin, since for the analysis of the disparity at least two taxa must be present in each considered interval. The distribution of taxa in the different time bins was based on the time calibrated tree of Pteraspidiformes heterostracans provided by Randle & Sansom (2017a, p. 595, fig. 7); the occurrence of taxa for each time bins is reported in supplementary material (Appendix 1).

Taxic diversity for Pteraspidiformes heterostracans is simply the sum of taxa in each time bin. Two disparity analyses were conducted; one on the classical discrete characters (including discretised quantitative characters) and the second, using the continuous characters only. Disparity was calculated both as the total variance and as the sum of ranges for the two different datasets (discrete and continuous). According to several authors (Foote, 1997; Erwin, 2007; Ruta, 2009; Prentice, Ruta, & Benton, 2011) disparity as total variance indicates essentially how the considered taxa are dispersed in the morphospace, whereas disparity as sum of ranges represents a good indication of the total occupied morphospace through time (see Wills, Briggs, & Fortey, 1994; Prentice, Ruta, & Benton, 2011). These indications must be carefully taken into account in the interpretation of the results obtained with the study (see below).

Disparity analysis of the discrete dataset (65 discrete characters) (Randle & Sansom, 2017a) was subjected to a Principal Coordinates Analysis on the free software PAST 3.10 (Hammer, Harper, & Ryan 2001), using the ‘Gower’ similarity index (c=2 Transformation Exponent), preferable to the simple Euclidean distance (see Hammer, 2013). Coding for the discreet character 42 in *Helaspis* and *Psephaspis* has been replaced by a question mark being polymorphic in the two taxa (two states of the character present). The PCO scores were used to calculate disparity, both as total variance and as sum of ranges, for the discrete character dataset (see Appendix 1 in the supplementary material). Only the first 23 principal coordinates were considered in the results, as the 24th was constant, not contributing to disparity.

22 continuous characters from Randle and Sansom (2017a) were analysed using a Principal Component Analysis, again using the software PAST 3.10. Missing entries were computed using the ‘iterative imputation’ in PAST, as suggested by Hammer (2013). Before the analysis, the raw data were log transformed for the correspondence of the log-transform to an isometric null hypothesis and to fit linear models (see Chinnery, 2004; Cheng et al., 2009; Romano & Citton, 2015; Romano & Citton, 2017; Romano, 2017a; Romano,2017b; Citton et al., 2017). Linear measures are in general preferable to ratios in Principal Component Analyses (see Hammer and Harper, 2006). However in this case the original ratios were used to perform the analysis, to be congruent with the results obtained by Randle & Sansom (2017a). Even in this case, the scores obtained from the 22 principal components were used to calculate disparity both as sum of ranges and variance (see Appendix 1).

RESULTS

The first occurrence of Pteraspidiformes heterostracans is in the Pridoli (Upper Silurian) with fairly low levels of diversity (Figs. 2A, green dotted line), and the clade is represented by just 4 genera. However, their diversity rises and attains its maximum in the Lochkovian to Pragian. From the Emsian onwards the number of taxa begins to decrease consistently until their demise in the Frasnian (Upper Devonian).

Disparity for the discrete-with-discretised characters (Fig. 2B) follow a very similar pattern to diversity, especially the sum of ranges. Disparity, as measured by total variance, begins to decrease in the Pragian, while ~~in~~ the sum of ranges disparity remains at the same level of the preceding time bin (i.e. Lochkovian). Sum of ranges disparity begins to decline from the Emsian onwards mirroring that~~’s~~ of diversity; however, disparity as total variance shows the same value for the Emsian and Eifelian after which it decreases abruptly until it reaches the minimum in the Givetian-Frasnian.

Similarly to the discrete characters the trend of disparity as sum of ranges for the continuous characters (Fig. 2C), closely matches the diversity through time except for a peak in the Pragian. Contrasting with the discrete characters, the continuous characters have high levels of disparity (for both sum of ranges and total variance) in the Pridoli. Disparity as total variance is decoupled with respect to diversity, with maximum disparity occurring at the beginning of their evolutionary history rather than in the Lochkovian, as seen in the discrete characters disparity. After this initial peak in the Pridoli, disparity declines until the Pragian and remains low until Givetian-Frasnian.

Morphospace occupation for the discrete-with-discretised characters and continuous characters through time can be seen in Fig. 3A. Maximum morphospace exploration (convex hull area) for the discrete-with-discretised characters is observed in the Lochkovian, which overlaps with morphospace occupied by Pteraspidiformes in the Pridoli and subsequent time bins (Pragian-Frasnian). Fig. 3B shows morphospace occupation of Pteraspidiformes as described by the continuous characters. There appears much more overlap in morphospace occupation through time bins than seen in the discrete-with-discretised characters, with one taxon extending morphospace occupation in the Pridoli. Throughout the majority of their history the Pteraspidiformes, occupy similar morphospace.

Fig. 4 shows the relative position of Pteraspidiformes taxa, grouped by family, in their Principal component analyses (continuous characters) and Principal coordinates (discrete characters) using the first two axes. There is much overlap in Pteraspidiformes morphospace using the continuous characters (Fig. ~~4A). Whereas~~, the discrete morphospace plot (Fig. 4B) there is much less overlap between the taxonomic groups. In particular, the Doryaspidae and Anchipteraspididae are very well separated, without overlap from the convex hulls of other families in the continuous character plot.

Other patterns seen in the classic cladistic character plot (Fig. 4A) include~~s~~ the Protopteraspididae overalpping with all the other convex hulls, with a truly substantial superimposition with the Anchipteraspididae, which in this case are not well separated from morphospaces explored by other groups. Another interesting result is that members of Psammosteidae do not cluster together in the graph, with *Psammosteus* occurring completely within the morphospace of the Doryaspidae. Many Pteraspidoidei *incertae sedis* fall within the convex hull identified by the families recognized by Randle & Sansom (2017a); the only taxa that fall outside a convex hull or the overlapping of several convex hulls are *Eucyclaspis*, *Parapteraspis*, and *Podolaspis*.

The scatter plot of the PCA conducted on discrete characters is shown in Fig. 4B. patterns include overlap between the Rhinopteraspididae and Protopteraspididae, with *Althaspis* occurring in the shared morphospace. A second overlap in morphospace occupation is observed in the ranges of Protaspididae and Protopteraspididae, with *Tuberculaspis* and *Lampraspis* falling well inside the morphospace of Protopteraspididae. Among the Pteraspidoidei *incertae sedis*, the taxa *Djurinaspis*, *Dnestraspis*, *Europrotaspis*, *Lamiaspis*, *Larnovaspis*, *Oreaspis*, *Pteraspis Semipodolaspis* and *Unarkaspis* are not included in any convex hull identified by the PCA; *Mylopteraspis*, *Eucyclaspis* fall within the Protaspididae; *Alaeckaspis*, *Blieckaspis*, *Eucyclaspis*, *Mylopteraspidella*, and *Protaspis* fall within the morphospace of

Protopteraspididae; *Parapteraspis* and *Pirumaspis* fall within the convex hull identified by the Rhinopteraspididae. Compared to the result obtained with the continuous characters (Principal Component Analysis), a greater and substantial separation is evident among the families of Pteraspidiformes in morphospace.

DISCUSSION

Generally diversity-disparity curves show that the disparity as sum of the ranges and total variance provide completely compatible and mostly superimposable macroevolution trends for classical discrete and continuous characters (Figs. 2). Greater correspondence is observed between diversity and disparity when disparity is calculated as the sum of ranges for discrete-with-discretised characters (Fig.2B). The only measure that does not show this trend is the total variance disparity obtained for the continuous characters (Fig. 2C). Considering total variance as a measure of the dispersion of taxa (Foote, 1997; Erwin, 2007; Ruta, 2009; Prentice, Ruta, & Benton, 2011), the result shows that for the continuous characters the maximum dispersion in the morphospace is found at the beginning of Pteraspidiformes evolutionary history (during the Pridoli); the dispersion then decreased consistently from the Lochkovian onwards. A possible explanation for this trend in the total variance could be the ‘early burst’ scenario. Mongiardino Koch *et al*. (2017) suggest that an ‘early burst’ result can be spurious if obtained from cladistic discrete characters as these are biased towards obviating autapomorphic characters overestimating evolution at the base of a clade. We, however, identify this pattern in our continuous dataset, perhaps suggesting that any generalization must be taken with caution, and that different clades can react differently and peculiarly to disparity analysis.

For all the above, worthy of note is a brief discussion on the reliability of using classical discrete cladistic characters to investigate disparity trend in a clade. Anderson & Friedman (2012), on the base of an empirical study on early gnathostomes, highlighted possible inconsistencies between the signals obtained from discrete and morphometric characters. In particular, according to the ~~A~~uthors, the biggest issue with cladistic~~s~~ characters for disparity analyses derive from the exclusion of autapomorphies from the original matrix (as not informative for phylogeny), and of potentially undersampling 'noisy' homoplastic features. These elements could obviously lead to the loss of information to reconstruct the total morphospace of a group during its evolutionary history. However, the inconsistency of the results obtained on early gnathostomes by Anderson & Friedman (2012) is strictly related to specific functional variation in the clade, and not to the overall morphological disparity. In fact the same authors consider in general the disparity based on cladistics characters as “*an important and broadly applicable tool for quantitative paleobiological analyses*” (Anderson & Friedman, 2012, p. 1262), even if not really suitable for ecological and functional variation analyses. The fact that our analysis is not focused on a specific functional structure or ecological variation but on overall morphospace of the group, and considering that discrete and morphometric characters converge to the same macro-evolutionary signal (using the sum of ranges as indication of morphospace saturation), we are very confident about the ~~goodness~~ and solidity of the results obtained in the present contribution.

The results in general indicate that Pteraspidiformes heterostracans explored morphospace early in their evolutionary history (Pridoli-Lochkovian), with much of the subsequent variation in their dermal armour occurring as variation in the proportions of already evolved anatomical features (Fig.2 & 3). Considering the total variance as a measure of the dispersion of the taxa in morphospace (see Foote, 1997; Erwin, 2007; Ruta, 2009; Prentice, Ruta, & Benton, 2011) and the sum of ranges as an indication of the total occupied morphospace (see Wills, Briggs, & Fortey, 1994; Prentice, Ruta, & Benton, 2011), the results also indicate that the Pteraspidiformes increase in taxonomic diversity also corresponds to an increase in taxa dispersion in morphospace and morphologies. This is followed by a progressive decrease in taxic diversity and morphospace occupation from the Emsian until their demise in the Frasnian (Fig. 2).

Extending the classic diversity categories identified by Gould, Gilinsky, & German (1987) to morphospace exploration, the Pteraspidiformes constitute a “bottom-heavy clade”, i.e. a group where a high initial disparity decreasing over time is detected. The great initial disparity in this case does not coincide with the evolutive first appearance of the group but it is shifted by at least one stage forward. An early radiation with a maximal disparity at the beginning of the evolutionary story of a clade had been found empirically in the literature for example for blastozoans (Foote, 1992), brachiopods (Carlson, 1992; McGhee, 1995; Smith & Bunje, 1999), Neoproterozoic acritarchs (Huntley, Xiao, & Kowalewski, 2006), Palaeozoic gastropods (Wagner, 1995), and crinoids (Foote, 1994, 1995, 1999). In the same way, a decrease in occupied morphospace during the evolutionary history of a clade was found for example in Carboniferous ammonoiods (Saunders & Work, 1996; Saunders & Work, 1997), rostroconchs (Wagner, 1997) and Palaeozoic stenolaemate bryozoans (Anstey & Pachut, 1995).

The discrete and continuous characters display differing patterns of overall morphospace occupation for the different taxonomic groups (Fig. 4). The continuous characters displays much overlap of taxonomic groups in morphospace, whereas, the discrete dataset show separate morphospace occupation for the families recognized by Randle & Sansom (2017a), apart from a slight overlap in the convex hulls of Protaspididae and Protopteraspididae, and between Protopteraspididae and Rhinopteraspididae

CONCLUSIONS

In this paper we present the first disparity (explored morphospace) versus diversity (number of taxa) analysis of Pteraspidiformes heterostracans using continuous and discrete characters. Patterns of morphological disparity and taxic diversity are in accordance, both showing a rise to a peak in the Lochkovian followed by a gradual decline in the Middle-Late Devonian.

The Pteraspidiformes, unlike other groups of heterostracans (i.e. Cyathaspididae and Traquairaspididae) arose later in the evolutionary history of the Heterostraci (the first heterostracans are from the Wenlock) (Randle & Sansom, 2017a; Ball & Dineley, 1963; Dineley & Loeffler, 1976). Therefore, it is unlikely that the early history of the Pteraspidiformes clade is lost due to fossil record or other abiotic biases, such as sea-level, as seen with other ostracoderm clades (Sansom, Randle & Donoghue, 2015). There is good correspondence between maximum taxonomic diversity and saturation of occupied morphospace, identifying the Pteraspidiformes heterostracans as a ‘bottom’ heavy clade, with most structural ‘bauplans’ and major morphologies already explored by the group in the Early Devonian.

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REFERENCES

Al-Sabouni N, Kucera M, Schmidt DN. 2007. Vertical niche separation control of diversity and size disparity in planktonic foraminifera. *Marine Micropaleontology* **63**:75–90.

Anderson PS, Friedman M. 2012. Using cladistic characters to predict functional variety: experiments using early gnathostomes. Journal of Vertebrate Paleontology **32**: 1254–1270.

Anstey AL, Pachut JF. 1995. Phylogeny, diversity history and speciation in Paleozoic bryozoans. 239–284. In Erwin, D. H. and Anstey, A. L. (eds). New approaches to speciation in the fossil record. Columbia University Press, New York, NY, 288 pp.

Bapst DW, Bullock PC, Melchin MJ, Sheets HD, Mitchell CE. 2012. Graptoloid diversity and disparity became decoupled during the Ordovician mass extinction. *Proceedings of the National Academy of Sciences* **109**: 3428–3433.

Benson RB, Evans M, Druckenmiller PS. 2012. High diversity, low disparity and small body size in plesiosaurs (Reptilia, Sauropterygia) from the Triassic–Jurassic boundary. *PLoS One* **7**: e31838.

Blieck ARM. 1984. Les Heterostraces Pteraspidiformes: systemastique, phylogenie, biostratigraphie et biogeographie. *Cahiers de Paléontologie*, 1–205.

Blieck ARM, Elliott DK, Gagnier PY. 1991. Some questions concerning the phylogenetic relationships of heterostracans, Ordovician to Devonian jawless vertebrates. In: Mee-Mann C, Yu-hai L, Zhang G eds. Early vertebrates and related problems of evoltionary biology (Intern. Symp. Beijing, 1987). Beijing: Science Press, 1–17.

Blieck ARM, Tarrant PR. 2001. *Protopteraspis gosseleti* (Vertebrata: Pteraspidimorphi: Heterostraci) from the Lower Devonian of Shropshire, England. *Palaeontology* **44:** 95–112.

Carlson SJ. 1992. Evolutionary trends in the articulate brachiopod hinge mechanism. *Paleobiology* **18(3)**:344–366.

Cheng YN, Holmes R, Wu XC, Alfonso N. 2009. Sexual dimorphism and life history of *Keichousaurus hui* (Reptilia: Sauropterygia). *Journal of Vertebrate Paleontology* **29**:401–408.

Chinnery B. 2004. Morphometric analysis of evolutionary trends in the ceratopsian postcranial skeleton. *Journal of Vertebrate Paleontology* **24**:591–609.

Citton P, Romano M, Salvador I, Avanzini M. 2017. Reviewing the upper Pleistocene human footprints from the 'Sala dei Misteri'in the Grotta della Bàsura (Toirano, northern Italy) cave: An integrated morphometric and morpho-classificatory approach. *Quaternary Science Review* **169**:50–64.

Colombo M, Damerau M, Hanel R, Salzburger W, Matschiner M. 2015. Diversity and disparity through time in the adaptive radiation of Antarctic notothenioid fishes. *Journal of Evolutionary Biology* **28**:376–394.

Davis SP, Finarelli JA, Coates MI. 2012. Acanthodes and shark like conditions in the last common ancestor of modern gnathos tomes. *Nature* **486**:247–250.

Deline B, Ausich WI. 2011. Testing the plateau: a reexamination of disparity and morphologic constraints in early Paleozoic crinoids. *Paleobiology* **37**:214–236.

Donoghue PCJ, Keating JN. 2014. Early vertebrate evolution. *Palaeontology* **57**:879–893. DOI: 10.1111/pala.12125.

Eble GJ. 2000. Contrasting evolutionary flexibility in sister groups: disparity and diversity in Mesozoic atelostomate echinoids. *Paleobiology* **26**:56–79.

Erwin DH. 2007. Disparity: morphological pattern and developmental context. *Palaeontology* **50**:57–73.

Foote M. 1992. Paleozoic record of morphological diversity in blastozoan echinoderms. *Proceedings of the National Academy of Sciences* **89**:7325–7329.

Foote M. 1994. Morphological disparity in Ordovician-Devonian crinoids and the early saturation of morphological space. *Paleobiology* **20**:320–344.

Foote M. 1995. Morphology of Carboniferous and Permian crinoids. *Contributions from the Museum of Paleontology, University of Michigan* **29**:135–184.

Foote M. 1996. Ecological controls on the evolutionary recovery of post-Paleozoic crinoids. *Science* **274**:1492–1495.

Foote M. 1997. Sampling, taxonomic description, and our evolving knowledge of morphological diversity. *Paleobiology* **23**:181–206.

Foote M. 1999. Morphological diversity in the evolutionary radiation of Paleozoic and post-Paleozoic crinoids. *Paleobiology* **25**:1–116.

Foth C, Brusatte S, Butler R. 2012. Do different disparity proxies converge on a common signal? Insights from the cranial morphometrics and evolutionary history of Pterosauria (Diapsida: Archosauria). *Journal of evolutionary biology* **25**: 904–915.

Glaubrecht M, Brinkmann N, Pöppe J. 2009. Diversity and disparity ‘down under’: Systematics, biogeography and reproductive modes of the ‘marsupial’freshwater Thiaridae (Caenogastropoda, Cerithioidea) in Australia. *Zoosystematics and Evolution* **85**:199–275.

Gould SJ, Gilinsky NL, German RZ. 1987. Asymmetry of lineages and the direction of evolutionary time. *Science* **236**:1437–1441.

Halliday TJD, Goswami A. 2016. Eutherian morphological disparity across the end-Cretaceous mass extinction. *Biological Journal of the Linnean Society* **118**:152–168.

Hammer Ø. 2013. PAST Paleontological Statistics Version 3.0: Reference Manual. University of Oslo.

Hammer Ø, Harper DAT, Ryan PD. 2001. PAST: paleontological statistics software package for education and data analysis. *Palaeontol Electron* **4**, 9.

Hetherington AJ, Sherratt E, Ruta M, Wilkinson M, Deline B., Donoghue PCJ. 2015. Do cladistic and morphometric data capture common patterns of morphological disparity? *Palaeontology* **58**: 393–399.

Hopkins MJ. 2013. Decoupling of taxonomic diversity and morphological disparity during decline of the Cambrian trilobite family Pterocephaliidae. *Journal of Evolutionary Biology* **26**:1665–1676.

Huntley JW, Xiao SH, Kowalewski M. 2006. 1.3 billion years of acritarch history: an empirical morphospace approach. *Precambrian Research* **144**:52–68.

Klingenberg CP, Gidaszewski NA. 2010. Testing and quantifying phylogenetic signals and homoplasy in morphometric data. *Systematic Biology* **59**: 245–261.

Ilyes RR., Elliott DK. 1994. New Early Devonian pteraspidids (Agnatha, Heterostraci) from East-Central Nevada. *Journal of Paleontology* **68**:878–892.

Janvier P. 1996. Early Vertebrates. New York: Oxford University Press Inc.

Larson DW, Brown CM, Evans DC. 2016. Dental disparity and ecological stability in bird-like dinosaurs prior to the end-Cretaceous mass extinction. *Current Biology* **26**:1325–1333.

Lefebvre B, Eble GJ, Navarro N, David B. 2006. Diversification of atypical Paleozoic echinoderms: a quantitative survey of patterns of stylophoran disparity, diversity, and geography. *Paleobiology* **32**:483–510.

Lofgren AS, Plotnick RE, Wagner APJ. 2003. Morphological diversity of Carboniferous arthropods and insights on disparity patterns through the Phanerozoic. *Paleobiology* **29**:349–368.

Marx FG, Fordyce RE. 2015. Baleen boom and bust: a synthesis of mysticete phylogeny, diversity and disparity. *Royal Society Open Science* **2**:140434.

McGhee G.R. Jr 1995. Geometry of evolution in the biconvex Brachiopoda: morphologic effects of mass extinction. *Neues Jahrbuch fur Geologie und Palaontologie-Abhandlungen* **197**:357–382.

MacLeod N. 2002. Phylogenetic signals in morphometric data. 100–138. In MacLeod N., Forey P.L. (eds.). Morphology, Shape and Phylogeny. Taylor & Francis Inc., New York, NY.

Mongiardino Koch N, Ceccarelli FS, Ojanguren-Affilastro AA, Ramírez MJ. 2017. Discrete and morphometric traits reveal contrasting patterns and processes in the macroevolutionary history of a clade of scorpions. *Journal of evolutionary biology* **30:**814–825.

Pernègre VN. 2002. The genus Doryaspis White (Heterostraci) from the Lower Devonian of Vestspitsbergen, Svalbard. *Journal of Vertebrate Paleontology* **22**:735–746.

Pernègre VN, Elliott DK 2008. Phylogeny of the Pteraspidiformes (Heterostraci), Silurian Devonian jawless vertebrates. *Zoologica Scripta* **37**,391–403. DOI: 10.1111/j.1463-6409.2008.00333.x.

Pernègre VN, Goujet D. 2007. The Genus Gigantaspis Heintz, 1962 (Vertebrata, Heterostraci) from the Lower Devonian of Spitsbergen. *Palaeontology* **50**,323–346. DOI: 10.1111/j.1475-4983.2007.00638.x.

Prentice KC, Ruta M, Benton MJ. 2011. Evolution of morphological disparity in pterosaurs. *Journal of Systematic Palaeontology* **9**:337–353.

Randle E, Sansom RS. 2016. Exploring phylogenetic relationships of Pteraspidiformes heterostracans (stem- gnathostomes) using continuous and discrete characters. *Journal of Systematic Palaeontology*, DOI: 10.1080/14772019.2016.1208293.

Randle E, Sansom RS. 2017a. Exploring phylogenetic relationships of Pteraspidiformes heterostracans (stem-gnathostomes) using continuous and discrete characters. *Journal of Systematic Palaeontology* **15(7)**:583–599.

Randle E, Sansom RS. 2017b. Phylogenetic relationships of the "higher heterostracans" (Heterostraci: Pteraspidiformes and Cyathaspididae), extinct jawless vertebrates. *Zoological Journal of the Linnean Society* **181(4)**:910–926.

Romano M. 2017a. Disparity vs. diversity in Stegosauria (Dinosauria, Ornithischia): cranial and post-cranial sub-dataset provide different signals. *Historical Biology*, DOI: 10.1080/08912963.2017.1397655.

Romano M. 2017b. Long bone scaling of caseid synapsids: a combined morphometric and cladistic approach. *Lethaia* **50(4)**:511–526, http://dx.doi.org/10.1111/let.12207.

Romano M, Citton P. 2015. Reliability of digit length impression as a character of tetrapod ichnotaxobase: considerations from the Carboniferous–Permian ichnogenus *Ichniotherium*. *Geological Journal* **50**:827–838.

Romano M, Citton P. (2017). Crouching theropod at the seaside. Matching footprints with metatarsal impressions and theropod authopods: a morphometric approach. *Geological Magazine* **154(5)**:946–962.

Romano M, Brocklehurst N, Manni R, Nicosia U. 2018. Multiphase morphospace saturation in cyrtocrinid crinoids. *Lethaia*, DOI:10.1111/let.12276.

Romano M, Brocklehurst N, Fröbisch J. 2017. Discrete and continuous character-based disparity analyses converge to the same macroevolutionary signal: a case study from captorhinids. *Scientific Reports* **7(1)**:17531, DOI: 10.1038/s41598-017-17757-5.

Ruta M. 2009. Patterns of morphological evolution in major groups of Palaeozoic Temnospondyli (Amphibia: Tetrapoda). *Special Papers in Palaeontology* **81**:91–120.

Ruta M, Angielczyk KD, Fröbisch J, Benton MJ. 2013. Decoupling of morphological disparity and taxic diversity during the adaptive radiation of anomodont therapsids. *Prooceding Royal Society B* **280**:20131071.

Sansom RS. 2009. Endemicity and palaeobiogeography of the Osteostraci and Galeaspida: a test of scenarios of gnathostome evolution. *Palaeontology* **52**:1257–1273.

Sansom RS, Randle E, Donoghue PC. 2015. Discriminating signal from noise in the fossil record of early vertebrates reveals cryptic evolutionary history. *Proceedings of the Royal Society of London B: Biological Sciences* **282(1800)**:20142245.

Saunders WB, Work DM. 1996. Shell morphology and suture complexity in Upper Carboniferous ammonoids. *Paleobiology* **22(2)**:189–218.

Saunders WB, Work DM. 1997. Evolution of shell morphology and suture complexity in Paleozoic prolecanitids, the rootstock of Mesozoic ammonoids. *Paleobiology* **23(3)**:301–325.

Scholz H, Hartman JH. 2007. Paleoenvironmental reconstruction of the Upper Cretaceous Hell Creek Formation of the Williston Basin, Montana, USA: Implications from the quantitative analysis of unionoid bivalve taxonomic diversity and morphologic disparity. *Palaios* **22**:24–34.

Smith LH, Bunje PM. 1999: Morphologic diversity of inarticulate brachiopods through the Phanerozoic. *Paleobiology* **25**:396–408.

Villier L, Eble GJ. 2004. Assessing the robustness of disparity estimates: the impact of morphometric scheme, temporal scale, and taxonomic level in spatangoid echinoids. *Paleobiology* **30**:652–665.

Wagner PJ. 1995. Diversity patterns among early gastropods: contrasting taxonomic and phylogenetic descriptions. *Paleobiology* **21**:410–439.

Wagner PJ. 1997. Patterns of morphologic diversification among the Rostroconchia. *Paleobiology* **23(1)**:115–150.

Whiteside JH, Ward PD. 2011. Ammonoid diversity and disparity track episodes of chaotic carbon cycling during the early Mesozoic. *Geology* **39**:99–102.

Wills MA, Briggs DEG, Fortey RA. 1994. Disparity as an evolutionary index: a comparison of Cambrian and Recent arthropods. *Paleobiology* **20**:93–131.

White, E. I. 1935. The ostracoderm Pteraspis Kner and the rela- tionships of the agnathous vertebrates. Philosophical Trans- actions of the Royal Society of London, Series B, 225, 381-457.

Figure captions

Figure 1. (A) Dorsal shield of *Protopteraspis sartoki* NMC.13869 (National Museum of Canada, Ottawa, Canada) a Protopteraspididae Pteraspidiformes. (B) Ventral view of *Errivaspis waynensis* P.17479 (Natural History Museum, London, UK) a Rhinopteraspididae Pteraspidiformes. (C) Dorsal view of *Cosmaspis transversa* PF4924 (Field Museum, Chicago, USA) a Protaspididae Pteraspidiformes. (D) Pteraspidiformes anatomy. (E) Reconstruction cartoons of the main Pteraspidiformes groups and general morphologies. Scale bar – 10mm. Rhinopteraspididae – Blieck 1981, Anchipteraspididae Elliott 1984, Protopteraspididae Blieck & Tarrant 2001.

Figure 2. (A) Pteraspidiformes taxic diversity through time, (B) disparity of Pteraspidiformes heterostracans using discrete-with-discretised characters (both total variance and sum of ranges), (C) disparity of Pteraspidiformes heterostracans using continuous characters (both total variance and sum of ranges).

Figure 3. Morphospace occupation through time in Pteraspidiformes heterostracans for the (A) discrete-with-discretised characters, and (B) continuous characters.

Figure 4. Scatter plots of first two principal components and principal coordinates performed respectively on (A) continuous characters (B) discrete-with-discretised characters. Taxonomic assignment following Randle & Sansom (2017a), with references to taxonomic groups in Figure 1.

Figure 1

Figure 1

(A) Dorsal shield of *Protopteraspis sartoki* NMC.13869 (National Museum of Canada, Ottawa, Canada) a Protopteraspididae Pteraspidiformes. (B) Ventral view of *Errivaspis waynensis* P.17479 (Natural History Museum, London, UK) a Rhinopteraspididae Pteraspidiformes. (C) Dorsal view of *Cosmaspis transversa* PF4924 (Field Museum, Chicago, USA) a Protaspididae Pteraspidiformes. (D) Pteraspidiformes anatomy. (E) Reconstruction cartoons of the main Pteraspidiformes groups and general morphologies. Scale bar – 10mm. Rhinopteraspididae – Blieck 1981, Anchipteraspididae Elliott 1984, Protopteraspididae Blieck & Tarrant 2001.

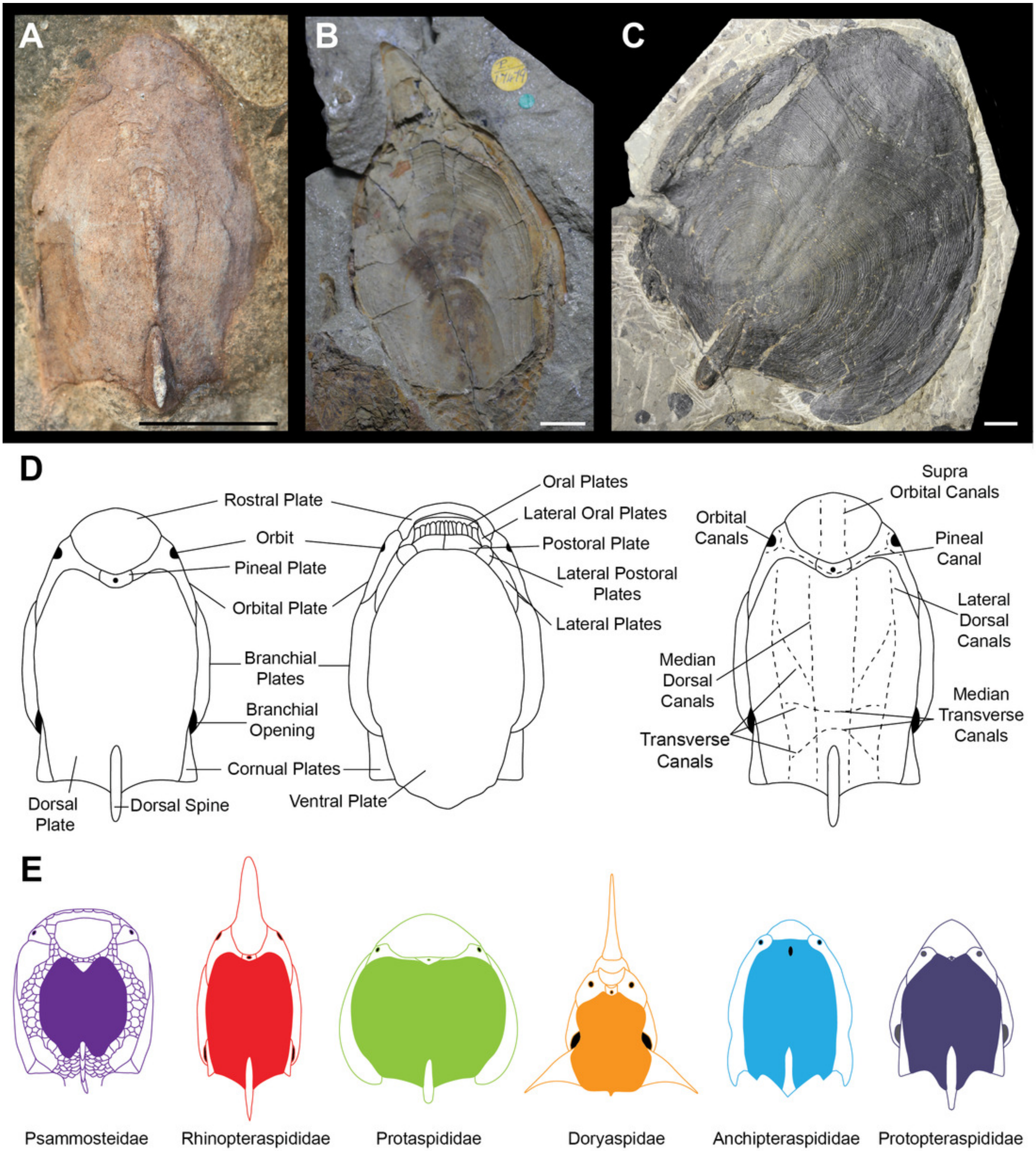

A
B
C
D
Rostral Plate
Orbit
Pineal Plate
Orbital Plate
Branchial Plates
Branchial Opening
Cornual Plates
Dorsal Plate
Dorsal Spine
Ventral Plate
Oral Plates
Lateral Oral Plates
Postoral Plate
Lateral Postoral Plates
Lateral Plates
Supra Orbital Canals
Orbital Canals
Pineal Canal
Lateral Dorsal Canals
Median Dorsal Canals
Median Transverse Canals
Transverse Canals
E
Psammosteidae
Rhinopteraspididae
Protaspididae
Doryaspidae
Anchipteraspididae
Protopteraspididae

Figure 2

Figure 2

Diversity (number of taxa) vs. disparity (both as total variance and sum of ranges) in Pteraspidiformes heterostracans calculated on the base of continous characters from Randle & Sansom (2017a). Diversity: green dotted line; Disparity: red solid line.

Note: Auto Gamma Correction was used for the image. This only affects the reviewing manuscript. See original source image if needed for review.

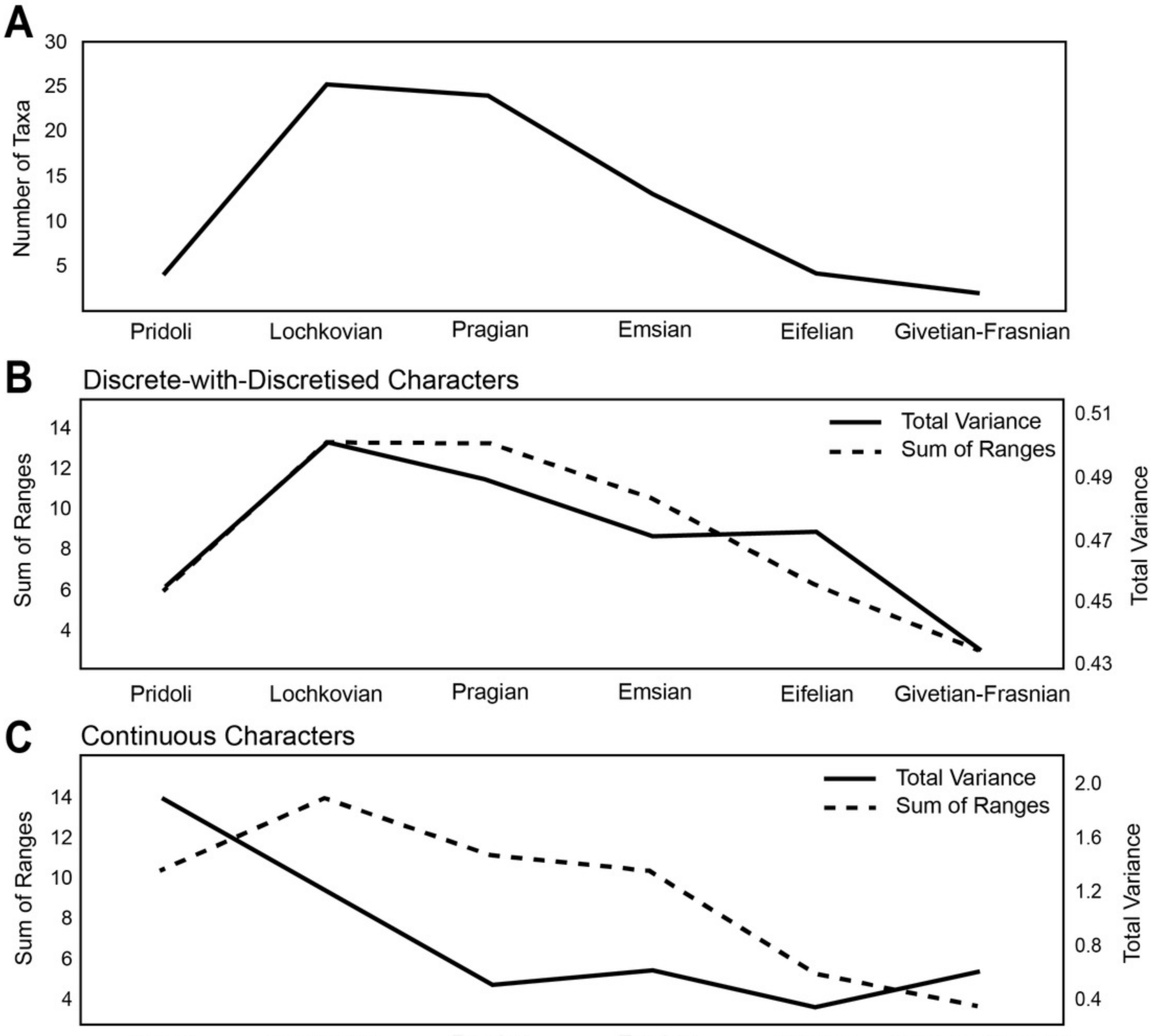


Figure 3

Figure 3

Morphospace occupation through time in Pteraspidiformes heterostracans for the (A) discrete-with-discretised characters, and (B) continuous characters.

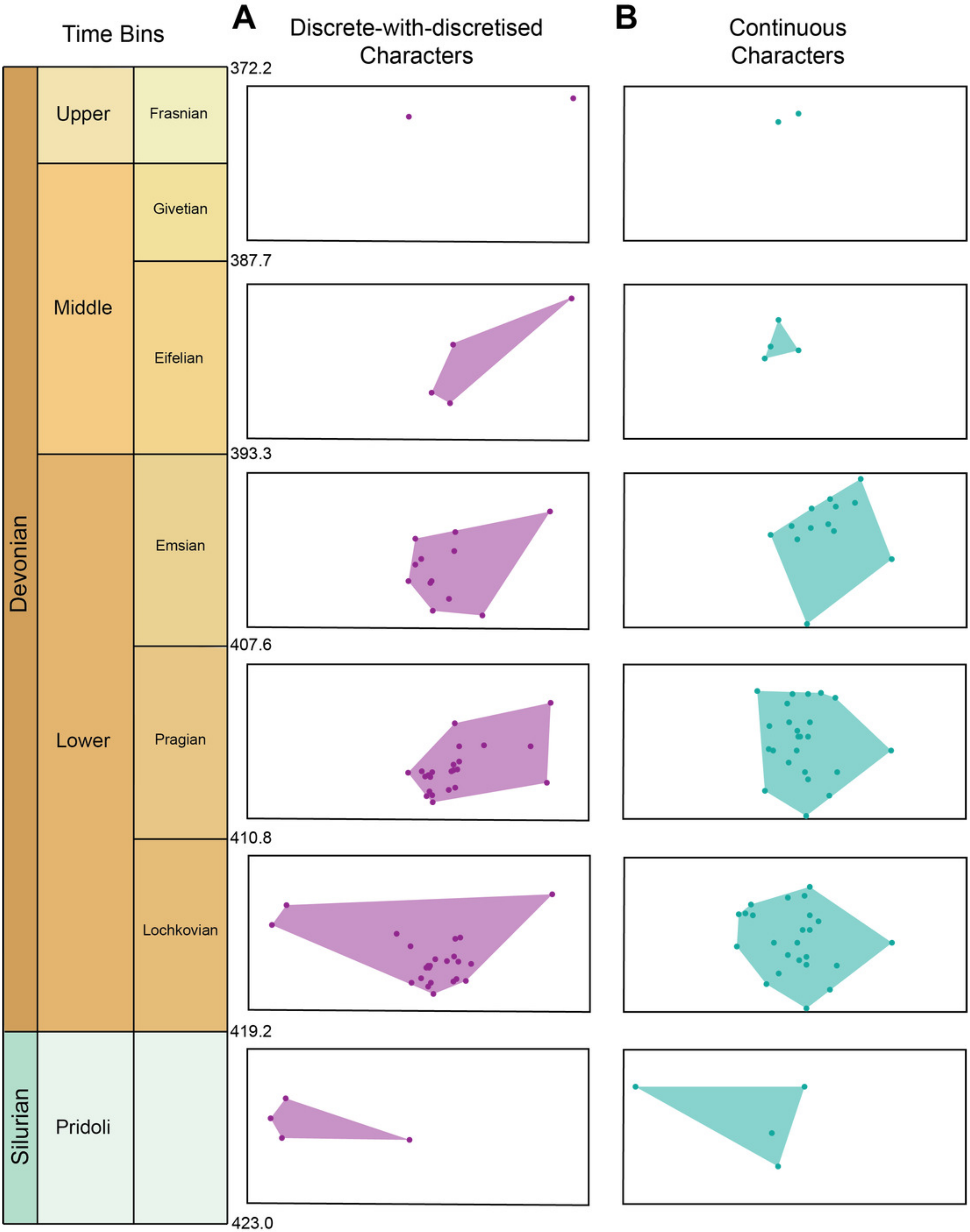
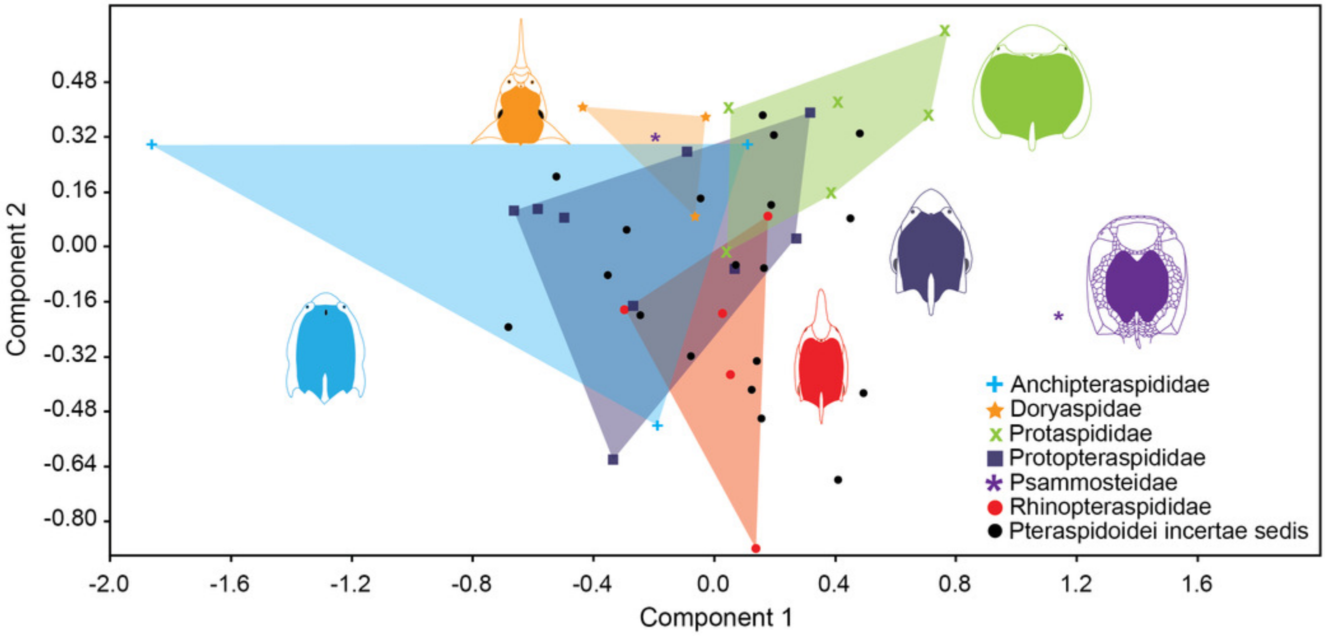

Time Bins
A
Discrete-with-discretised Characters
B
Continuous Characters
Devonian
Silurian
Upper
Middle
Lower
Pridoli
Frasnian
Givetian
Eifelian
Emsian
Pragian
Lochkovian
372.2
387.7
393.3
407.6
410.8
419.2
423.0

Figure 4

Figure 4

Scatter plots of first two principal components performed on continuous characters (A) and first two principal coordinated on discrete characters (B). The group are named following Randle & Sansom (2017a).

A Discrete-with-Discretised Characters



B Continuous Characters