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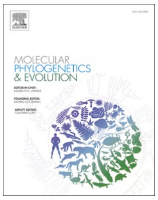

Mesozoic origin of coleoid cephalopods and their abrupt shifts of diversification patterns

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ABSTRACT

Coleoids are the most diverse group of cephalopod mollusks. While their origin is date during the Mesozoic, the diversification pattern is unknown. However, two hypotheses have been proposed. The first suggests an increasing diversification rate after the Cretaceous–Paleogene extinction event (K–Pg) as consequence of empty habitats left by the ammonites and belemnites. The second hypothesis proposes a mid-Cenozoic increase in diversification rate related to distributional changes during ice ages and biotic interactions. To test these hypotheses, we estimated a lineage through time (LTT) and the gamma-statistic along with model-based diversification rates. These analyses were conducted on a dated molecular phylogeny for coleoids that we reconstructed using five molecular markers (cytochrome *b*, 16S rRNA, cytochrome oxidase I, rhodopsin, and PAX-6). Our divergence time estimation suggests that coleoids originated in the Mesozoic Era (Middle Triassic) and that both main clades (Decapodiformes and Octopodiformes) diverged in the Cretaceous/Jurassic Period. The LTT, gamma statistic, and diversification rates inferred with the Bayesian Analysis of Macro-evolutionary Mixtures (BAMM), indicate an acceleration in diversification rate over time since the origin of coleoids. Additionally, BAMM allowed us to detect abrupt increases in diversification rate before and after the K-Pg boundary. Our results partially support both hypotheses as all analyses indicate that the coleoid diversification rate was increasing during the Cenozoic. However, our results also indicate increasing diversification rates before the K-Pg boundary. We propose that the radiation of coleoids has been shaped by an acceleration in diversification rate over time, including exceptional episodes of abrupt increases before and after the K-Pg boundary.

1. Introduction

Among cephalopods, the subclass Coleoidea is the most diverse and abundant lineage containing over 800 described species (Hoving et al., 2014; Allcock et al., 2015; Jain, 2017). Coleoids have an internal shell (sometimes absent), 8 or 10 circumoral appendages, and a pair of ctenidia (Jereb et al., 2010; Hanlon et al., 2018). These cephalopods have a wide distribution in all oceans – from the poles to the tropics – on continental margins and in oceanic areas (Hanlon and Messenger, 1996; Jereb and Roper, 2005). Coleoids represent the majority of the diversity of modern cephalopods and constituted an important part of the Paleozoic nekton (Kröger 2005).

Coleoids are considered monophyletic based on morphological and molecular data (Carlini and Graves, 1999; Carlini et al., 2000; Vecchione et al., 2000; Lindgren et al., 2004; Strugnell et al., 2005; Strugnell and Nishiguchi, 2007; Allcock et al., 2011; 2015; Lindgren et al., 2012;

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Strugnell et al., 2017; Lindgren and Anderson, 2018) and subdivided into two main clades: Decapodiformes (squids, bobtail squids and cuttlefishes) and Octopodiformes (vampire squid, cirrate and incirrate octopods). Nonetheless, some of the relationships among major taxa within each superorder are complex (specially in Decapodiformes) and continue to be the subject of ongoing debate (Nishiguchi and Mapes, 2008; Lindgren et al., 2012; Sanchez et al., 2018, Anderson and Lindgren, 2021).

According to the fossil record, cephalopods originated in the Early Cambrian period (∼530 Mya) from a monoplacophoran-like mollusk (Ward and Bandel, 1987; Mutvei et al., 2007; Kröger et al., 2011) that evolved quickly, possibly due to its ability to regulate buoyancy, and that diversified into several lineages during the Ordovician (Kröger, 2005). Paleontological records dating from the Early Carboniferous (∼330 Mya) suggest an origin of the subclass Coleoidea from Devonian Bactritoidea (Nishiguchi and Mapes, 2008; Kröger et al., 2011; Klug et al., 2019). In addition, the internalization and reduction of the mineralized shell could favour the diversification of coleoids at the end of the Paleozoic (∼276 Mya) into the two main lineages, Octopodiformes and Decapodiformes (Boletzky, 1999; Young et al., 1998; Boyle and Rodhouse, 2005).

The molecular divergence timing of the Cephalopoda has been estimated several times in previous research (e.g., Strugnell et al., 2006; Kröger et al., 2011; Tanner et al., 2017; Uribe and Zardoya, 2017; Sanchez et al., 2018). Strugnell et al. (2006) were the first authors to use both molecular and fossil data to estimate divergence times for taxa within coleoid cephalopods and suggested a much earlier (Paleozoic, ∼400 Mya) origin for Decapodiformes and Octopodiformes than previously estimated. However, recently, Tanner et al. (2017) suggest that cephalopods diverged during the Silurian–Devonian period (∼420 Mya), while coleoids trace their origin to the latest part of the Paleozoic Era. Tanner et al. (2017) also found an ancient origin of Octopodiformes, extending to the Early Mesozoic Era (∼220 Mya), and presented evidence suggesting that Decapodiformes diversified in the Jurassic Period (∼180 Mya). These divergences estimates highlighted that the modern diversity of coleoid cephalopods could have emerged during the Mesozoic marine revolution (Klug et al., 2010), a period also marked by the radiation of most jawed nektonic marine vertebrates. Thus, the coleoid radiation could have been strongly influenced by competition with Mesozoic fish, as well as by the predation pressure exerted by ichthyosaurs, mosasaurs, and plesiosaurs (Sato and Tanabe, 1998; Everhart, 2004; Lomax, 2010). This suggests that the origin of modern cephalopods could have been in part contingent upon ecological competition with marine vertebrates (Packard, 1972; Tanner et al., 2017).

Previous studies have provided two competing hypotheses for the diversification of coleoids. The first hypothesis suggests that a rapid diversification of coleoids began after the K–Pg boundary, related to the mass extinction of Mesozoic vertebrates (Packard, 1972; Aronson, 1991). According to this hypothesis, the meteorite impact that occurred ∼ 65 Mya, marking the transition from the Late Cretaceous to the Paleogene (K–Pg), would have caused a violent global change in terrestrial and marine ecosystems (Alvarez et al., 1980; Norris et al., 1999). The K–Pg mass extinction accounts for the disappearance of about 75% of vertebrates (Archibald, 2012). However, in the seas, this event would have enabled vertebrates –such as ray-finned fishes (Acanthopterygii)– to diversify (Friedman, 2010; Near et al., 2013; Amorim and Costa, 2018). For marine invertebrates, the K–Pg event caused the complete extinction of ammonites and belemnites (Surlyk and Nielsen, 1999; Sole et al., 2002; Iba et al., 2011), which could have led to the diversification of contemporary coleoid cephalopods. If this is the case, then the increase in coleoid diversification rates could be associated with a decreased competition pressure resulting from the disappearance of predators, the empty habitats left by their competitors, and a greater adaptive plasticity (Solé et al., 2002; Lockwood, 2004).

The second hypothesis suggests an increase in coleoids diversification specifically in the mid Cenozoic (∼30 Mya), during ice ages related to the distributional changes and adaptation to the new climate conditions (e.g. cold waters) associated with biotic interactions (Nesis, 1978; 2003). This hypothesis is based on the fact that in the mid Cenozoic, the competition between cephalopods and fish, without many top predators to contend with, could have driven a much broader ecological diversification of coleoids. This could help explain why both coleoids and ray-finned fishes have achieved such great evolutionary success. Moreover, other research indicates that the main radiation of ray-finned fishes (Actinopterygii) began in the Cenozoic after K–Pg boundary and not in the Mesozoic (Sibert and Norris, 2015).

Several studies have inferred a rapid diversification of coleoids during the Cenozoic, which is attributed to the filling of the empty habitats left by the ammonites and belemnites (Lewy, 1999; Clarke, 2003; Fuchs and Lukeneder, 2014; Clements et al., 2017). Furthermore, coleoids refined jetting during the Cenozoic compared with coleoids from the Mesozoic (Fuchs & Iba, 2015; Fuchs et al., 2016), which could have allowed them to quickly colonize the empty habitats. The loss of calcification through coleoid evolution generated a change in their buoyancy – from neutral to negative (Wells and O'Dor, 1991; Fuchs and Iba, 2015). These adaptations could have helped coleoids to evolve alternative modes of movement and/or improved jet propulsion efficiency, leading to increased species diversification.

In this study, our aim was to estimate the divergence times of coleoids and the timings of increase in coleoid diversification rates using a reconstructed dated molecular phylogeny. With regard to diversification, we tested the two hypotheses that pose that the increase in diversification rate occurred after the K-Pg boundary (∼65 Mya) or around the Mid-Cenozoic (∼30 Mya), and additionally, we tested whether there was an abrupt increase in diversification rate along the evolutionary history of coleoids through time.

2. Materials and methods

2.1. DNA sequencing

We assembled a sequence dataset of 190 species of cephalopods by merging nucleotide sequences from GenBank with new sequence data obtained in study. Our dataset spanned a broad diversity of cephalopods (including members of Sepiida, Spirulida, Oegopsida, Myopsida, Octopoda and Vampyromorpha, with two species of Nautilida as outgroups) (Table S1). Our assembled sequence dataset included three mitochondrial genes (cytochrome *b* (CYTB), 16S rRNA (16S) and cytochrome oxidase I (COI)) and two nuclear genes (rhodopsin (RHO) and PAX-6 (PAX6)).

DNA was extracted from 24 species following a saline extraction protocol (Aljanabi and Martinez, 1997) for mitochondrial genes (CYTB, 16S and COI). PCR amplification for the CYTB gene was conducted using Cef-H and Cef-L primers (Santaclara et al., 2007). For 16S and COI, PCR amplification was performed using the same primers employed by Allcock et al. (2008). Our PCRs contained 1 μl (50 ng) of DNA template, 2.5 μl of 10X buffer, 2 μl (2 mM) $MgCl_2$, 1 μl (100 μM) of dNTP, 0.5 μl (10 1 M) of a solution of each primer, and 1 unit of Taq-polymerase, with a final volume of 25 μl. We performed PCRs using a Bio-Rad MyCycler ™ thermocycler (Bio-Rad, Hercules, CA, USA). The cycle program was as follows: a preheating step of 3 min at 95 °C, then 35 cycles of 30 s at 95 °C, 40 s at 51° C for COI, 50° C for CYTB and 55° C for 16S, and 1 min and 30 s at 72 °C, followed by a final extension step of 7 min at 72 °C. PCR products were purified and sequenced by Macrogen Inc (Korea). We edited the bidirectional sequences using ProSeq v2.9 software (Filatov, 2002). We have accessioned all sequences generated for this study in GenBank (Table S1).

2.2. Phylogenetic analyses

We separately aligned the nucleotide sequences for each gene using Multiple Sequence Comparison by Log-Expectation (MUSCLE) with default parameters for gap insertion and gap extension (Edgar, 2004), implemented in the MEGA v7.0 software (Kumar et al., 2016). We evaluated sequence saturation using Xia's test implemented in DAMBE 5 software (Xia, 2013). Once aligned, we used Mesquite v3.10 (Maddison and Maddison, 2016) to concatenate our aligned sequences for each of the five genes (CYTB, 16S, COI, RHO, and PAX6) into a single partitioned matrix.

The phylogenetic relationships of coleoid cephalopods was inferred by means of Bayesian inference using MrBayes v3.2 (Ronquist et al., 2012). We identified the best-supported substitution model for each gene using jModelTest2 (Darriba et al., 2012) (Table S2). For coding genes (CYTB, COI, RHO, and PAX6) a codon partition scheme was applied with unlinked parameters. This scheme gave a total of 13 partitions. Bayesian analysis was conducted with four chains, each with 10 million generations, sampled every 1,000 generations. The first 10% of generations was discarded as burn-in, leaving a total of 9,001 trees sampled from the posterior probability distribution. From these trees, we computed a (50%) majority consensus tree. We also evaluated convergence to the posterior distribution and mixing of the MCMC using Tracer v1.6 (Rambaut et al., 2014). Effective Sample Sizes (ESS) > 200 were accepted.

To compare our results from Bayesian Inference (BI) obtained from MrBayes, we conducted a Maximum Likelihood (ML) analysis using the IQ-TREE v1.6.5 (Nguyen et al., 2015; Trifinopoulos et al., 2016). In this analysis, we used separate nucleotide substitutions models for each partition as determined by ModelFinder (Kalyaanamoorthy et al. 2017, Chernomor et al., 2016). ModelFinder determined the best substitution model for each codon partitions (position 1, 2 and 3) of coding genes (i.e., CYTB, COI, RHO, PAX6). This scheme for coding genes gave a total of 12 partitions. When adding the non-coding gene (16S) we obtained a final 13 partitions matrix for analysis (Table S3). The node support was assessed using 5,000 replicates of the ultrafast bootstrap approximation, as implemented in IQ-TREE v1.6.5 (Hoang et al., 2018).

2.3. Divergence times estimation

Divergence times was estimated using BEAST v1.10.4 (Suchard et al., 2018) for the partitioned data set (CYTB, 16S, COI, RHO, PAX6) employing the same substitution models used for each character set in MrBayes phylogenetic analyses. We also used three codon partitions for coding genes (position 1, 2 and 3) with unlinked parameters (substitution rates and base frequencies). These options were assigned in BEAUti v1.10.4 (Suchard et al., 2018). Both, strict and relaxed molecular clocks were ran under different models (uncorrelated lognormal, gamma, and exponential). We used a 'Yule' (i.e., pure-birth) model as tree prior, and then conducted 20,000,000 generations of MCMC, logging every 1,000 generations. After excluding the first 10% (i.e., 2,000,000 generations) as burn-in, we verified that our effective sample sizes (ESSs) were all $>$ 200 using Tracer software.

The molecular clock was adjusted using seven calibration points (Table S4). The first calibration point is the divergence of the Nautiloidea and the lineage estimated to have led to Coleoidea (*Bactrites*) from the lower Devonian (Pragian, ~408 Mya; Kröger and Mapes, 2007) with gamma distribution and the following parameters: offset = 408, shape = 2.0, scale = 3.0. The second calibration point is the split between Decapodiformes and Octopodiformes using the octopodiform genus *Germanoteuthis* from the middle Triassic (Ladinian, 236 Mya; Schweigert and Fuchs, 2012) with gamma distribution and the following parameters: offset = 236, shape = 2.0, scale = 3.0. The third calibration point is the split of Vampyromorpha and Octopoda using the genus *Loligosepia* from the early Jurassic (Sinemurian, 195 Mya; Fuchs and Weis, 2008) with gamma distribution and the following parameters: offset = 195, shape = 2.0, scale = 3.0. The fourth calibration point is the split between Spirulida and Oegopsida from the early Cretaceous (Barremian, 128 Mya) based on previous works (Tanner et al., 2017) with normal distribution and the following parameters: mean = 128, s.d. = 12.8 Mya. The fifth calibration point is the divergence of the incirrate crown group using the species *Styletoctopus annae* from the late Cretaceous (Cenomanian, 93 Mya; Fuchs et al., 2009) with gamma distribution and the following parameters: offset = 93, shape = 2.0, scale = 3.0. The sixth calibration point is the divergence of loliginid subgroups using the species *Loligo applegatei* from the early Eocene (Ypresian, 48 Mya; Clarke and Fitch, 1979) with gamma distribution and the following parameters: offset = 48, shape = 2.0, scale = 3.0. The seventh calibration point is the divergence of the Argonautoidea using the species *Obinautilus pulchelus* from the early Oligocene (Rupelian, 29 Mya; Kobayashi, 1954) with gamma distribution and the following parameters: offset = 29, shape = 2.0, scale = 1.0. We identified the best-supported model for the molecular clock (strict or relaxed) by Bayes Factors.

2.4. Assessing diversification rate hypotheses

To test the hypotheses, we performed several diversification analyses on our maximum clade credibility tree (MCCT), obtained from BEAST analyses. We also performed diversification analyses on alternative trees that represent different topological hypotheses. We used PHYTOOLS v0.6–99 (Revell 2012) and DIVERSITREE v0.9–9 (FitzJohn, 2012) in R v3.5.1 (R Core Team, 2020) to estimate the LTT, gamma statistic, and diversification rates, respectively. In addition, the diversification rate pattern was explored using BAMM v2.5 (Rabosky, 2014) to identified abrupt shift of diversification along the phylogeny.

We first tested deviation from a constant-rate pure-birth diversification process using the γ-statistic of Pybus and Harvey (2000), while controlling for incomplete taxon sampling via the Monte Carlo constant rates (MCCR) test with 5,000 simulations using PHYTOOLS. Our assumed sampling fraction is based on having sampled 188 out of 840 described species of coleoids (Hoving et al., 2014). We also compared the observed LTT plot to simulated LTTs assuming a pure-birth process with 10,000 iterations using the PHYTOOLS function 'pbtree', followed by a test of γ-statistic with the simulated pure-birth phylogenies.

Second, to estimate speciation and extinction rates from our MCCT, we used the Maximum Likelihood method employed by Nee et al. (1994) implemented in the PHYTOOLS 'fit.yule' and 'fit.bd' functions as follows: first fitting a Yule (pure-birth) model and then a birth–death model to our estimated tree. Both functions also take into account the incomplete taxon sampling of this study (188 of 840 described species; Hoving et al., 2014) using the method suggested by Stadler (2012).

Third, using DIVERSITREE, we designed and ran a Bayesian MCMC analysis of diversification (10,000 generations). We then visualized the posterior distribution of the speciation rate (λ) and extinction rate (μ). Additionally, we estimated the net diversification (r [$\lambda - \mu$]) and the ratio of extinction to speciation rates (ε [μ / λ]). We also estimated the LLT and the speciation and extinction rates on three different phylogenetic topologies. These alternative topologies were based on Strugnell et al. (2017), Tanner et al. (2017), and Anderson & Lindgren (2021). We obtained these topologies by forcing the monophyly of the orders of Decapodiformes in BEAST to test if the tree topology can affect our results.

Finally, we additionally tested the diversification hypotheses by inferring the diversification rates across all branches of the MCCT, using BAMM v2.5 (Rabosky, 2014). BAMM is specially designed to detect heterogeneity in evolutionary rates, and it assumes that the rate of diversification changes across phylogenetic branches given a Poisson process. BAMM explores many candidate models of diversification according to the data and enables us to estimate the *posterior* probability of each model. The diversification model can also account for abrupt shifts in rate, which brings the unique opportunity to test whether there was any significant increase in diversification rate during the mid-Cenozoic (hypothesis 2). We used the *prior* information obtained with the setBAMMpriors function in BAMMtools R package (Rabosky et al., 2014). We ran the BAMM analysis considering the species sampling fraction across every order of Coleoidea. To obtain the orders' sampling fraction we considered the number of recognized species per order given the World Register of Marine Species (WoRMS; see Table 2). We ran the four MCMC chains for 51 million generations, sampling each 50,000 generations on a random sample of 20 trees obtained from the *posterior* distribution of BEAST analyses. In addition, the analysis was ran on the random samples of trees to evaluate the effect of alternative topologies and divergence times on the inferred diversification rate patterns.

3. Results

3.1. Phylogenetic analysis

Xia's test found no saturation of coding genes (CYTB: $Iss = 0.562 < Iss.c = 0.713$, $P < 0.001$; COI: $Iss = 0.327 < Iss.c = 0.718$, $P < 0.001$; RHO: $Iss = 0.443 < Iss.c = 0.709$, $P < 0.001$; PAX6: $Iss = 0.245 < Iss.c = 0.683$, $P < 0.001$).

The consensus of 9,001 phylogenetic trees sampled from the posterior distribution using MCMC in MrBayes (Fig. S1) showed high posterior probability (PP) values (>0.95) for 136 of the 189 nodes (71.9%). Bootstrap values on the ML tree (Fig. S2) were high (>90%) in 150 of the 189 nodes (79.4%) and corresponded closely to the posterior probabilities obtained using MrBayes (Fig. 1). The ML tree from IQ-TREE exhibited the best topology, resolving the polytomies present in the BI tree with high bootstrap support (>90, Fig. S1). For this reason, and due to the high congruence between phylogenies (ML and BI), we present the ML tree with the node support data combined in a single tree, showing the ultrafast bootstrap values from ML and the posterior probability values from the BI in the nodes (Fig. 1).

The topology of the estimated tree shows three main groups: Clade 1 represented by subclass Coleoidea; Clade 2 consisted of the superorder Decapodiformes; and, finally, Clade 3 composed of the superorder Octopodiformes. Within Clade 2, we identified five subclades (Fig. 1): Sepiolida (Clade 4); Idiosepiida (Clade 5); Sepiida (Clade 6), Spirulida + Oegopsida (Clade 7); and Loliginidae (Clade 8) (Fig. 1). Within Clade 3, we noted a total of three primary subclades: Cirrata (Clade 9); Argonautoidea (Clade 10); and Octopodoidea (Clade 11) (Fig. 1).

3.2. Divergence times

In our divergence time estimation, we found that the model that best fitted our data was the relaxed uncorrelated molecular clock with lognormal distribution ($-\ln = 33491.41$, $BF > 0.5$). According to this model, the mean divergence time estimate for the crown node of Cephalopoda dates to the Early Devonian at 412.08 Mya (95% HPD: 408.14 – 419.51; Table 1, Fig. 2). The split between Decapodiformes and Octopodiformes was in the Middle Triassic at around 241.20 Mya (236.14 – 250.91; Table 1, Fig. 2). The Most Recent Common Ancestor (MRCA) of Decapodiformes was in the Early Cretaceous at 109.76 Mya (93.15– 127.31; Table 1, Fig. 2), Sepiolids began to diversify in the Late Cretaceous 68.51 Mya (51.15 – 91; Table 1, Fig. 2), Idiosepiids began to diversify in the Late Eocene 35.84 Mya (20.38 – 52.28; Table 1, Fig. 2), Sepiids began to diversify in the Late Cretaceous 68.75 Mya (54.45 – 81.88; Table 1, Fig. 2). Moreover, the MRCA between spirulids and oegopsids was in the Late Cretaceous 88.66 Mya (75.71 – 101.9; Table 1, Fig. 2), Oegopsid squids began to diversify in the Late Cretaceous 76.99 Mya (64.64 – 90.17; Table 1, Fig. 2), and the beginning of diversification for loliginid squids was in the Middle Paleocene 58.22 Mya (50.32 – 66.79; Table 1, Fig. 2). The split between Vampyromorpha and Octopoda was in the Early Jurassic 198.92 Mya (195.23 – 205.75; Table 1, Fig. 2), Cirrate octopods began to diversify in the Late Cretaceous 71.8 Mya (36.93 – 112.92; Table 1, Fig. 2), Incirrate octopods began to diversify in the Late Cretaceous 99.85 Mya (93.3 – 110.33; Table 1, Fig. 2), Argonautoid octopods began to diversify in the Late Eocene 39.46 Mya (32.63 – 46.52; Table 1, Fig. 2) and, finally, the beginning of diversification for the family Octopodoidea (without Eledonidae) was in the Late Cretaceous 91.32 Mya (80.47 – 103.16; Table 1, Fig. 2).

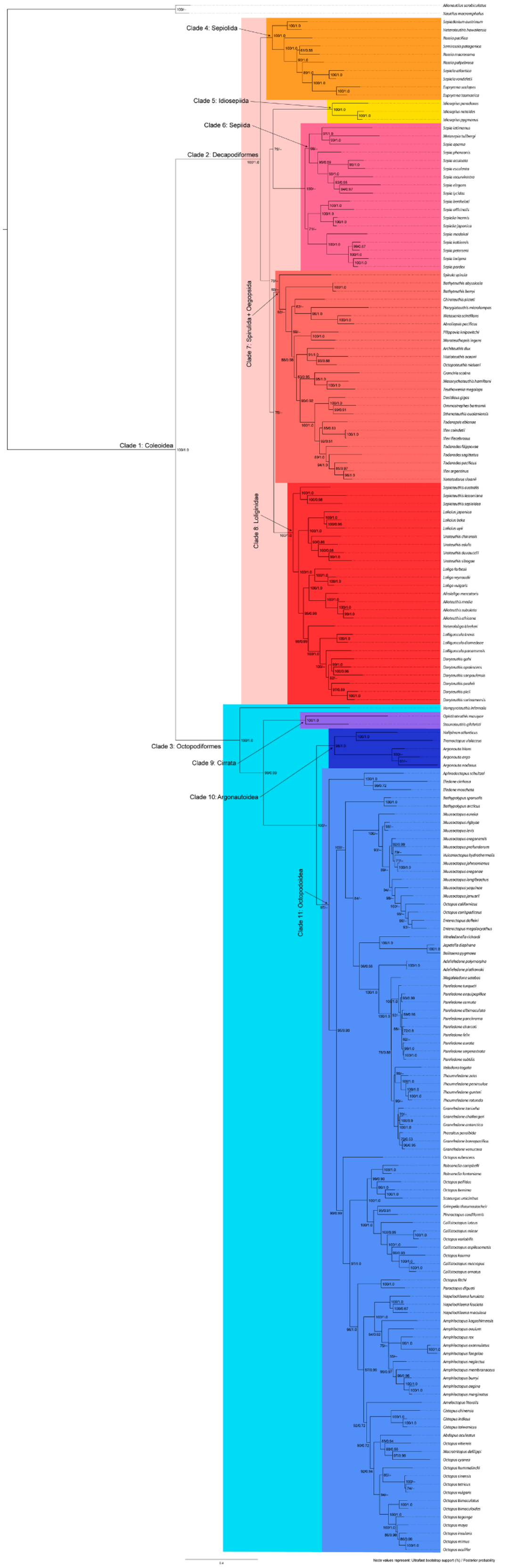

Fig. 1. Bayesian phylogram based on the majority rule consensus tree from 9,001 trees sampled from the posterior distribution using MCMC. Node values represent posterior probability/bootstrap support

Table 1
Estimated divergence time for each taxa in this study with their Highest posterior density (HPD 95%)

Taxa	Period	Median divergence time (Mya)	HPD 95% (Mya)
Cephalopoda	Early Devonian	412.08	408.14 – 419.51
Coleoidea	Middle Triassic	241.20	236.14 – 250.91
Decapodiformes	Early Cretaceous	109.76	93.15 – 127.31
Sepiolida	Late Cretaceous	68.51	51.15 – 91.00
Idiosepiida	Late Eocene	35.84	20.38 – 52.28
Sepiida	Late Cretaceous	68.75	54.45 – 81.88
Spirulida + Oegopsida	Late Cretaceous	88.66	75.71 – 101.90
Oegopsida	Late Cretaceous	76.99	64.64 – 90.17
Loliginidae	Late Paleocene	58.22	50.32 – 66.79
Octopodiformes	Early Jurassic	198.92	195.23 – 205.75
Cirrata	Late Cretaceous	71.80	36.93 – 112.92
Incirrata	Late Cretaceous	99.85	93.30 – 110.33
Argonautoidea	Middle Eocene	39.46	32.63 – 46.52
Octopodoidea	Late Cretaceous	91.32	80.47 – 103.16

Table 2
Orders' sampling fraction used for BAMM analyses.

Order	Number sampled species	Number of WoRMS recognized species	Sampling fraction used in BAMM
Idiosepiida	3	7	0.429
Myopsida	27	48	0.563
Oegopsida	25	266	0.094
Sepiida	18	120	0.150
Sepiolida	10	86	0.116
Spirulida	1	1	1.000
Octopoda	103	306	0.337
Vampyromorpha	1	1	1.000

3.3. *Assessing diversification rate hypotheses*

The observed LTT plot shows an exponential growth curve (Fig. 3; red line, Fig. S3); with a gamma value (γ = -0.9541) higher than the gamma values obtained from the null model distribution (γ = -5.6768 average) (Fig. S4). This result indicates an acceleration of lineage accumulation since the origin of Coleoidea. Moreover, according to corrected values of the γ-test statistic obtained by the MCCR test, the hypothesis of constant speciation under a Yule pure-birth model is strongly rejected (γ = -0.9541, $p < 0.001$). This result corroborates the pattern of variable diversification rate (increasing rate) during the radiation of coleoids. Considering these results, we can partially support the two guiding hypotheses of this study, as the coleoid diversification rate was increasing after the K-Pg boundary, during the Cenozoic, but our results show that diversification rate was also increasing before K-Pg, during the Mesozoic. In the best-fitting birth–death model, the ML speciation rate (λ) was estimated to be 0.119 lineages/Mya with an extinction rate (μ) of 0.086 lineages/Mya (Fig. S5). The birth–death model explained our estimated tree significantly better than the Yule or pure-birth model (LRT = -45.43, χ^2 = 27.46, $P < 0.001$). The LTT plots obtained from phylogenetic topologies given previous studies (Fig. S6) presented similar diversification patterns (Fig S7; S8; Table S5) – we found an increasing diversification rate pattern, since the origin of coleoids, across all alternative phylogenetic topologies.

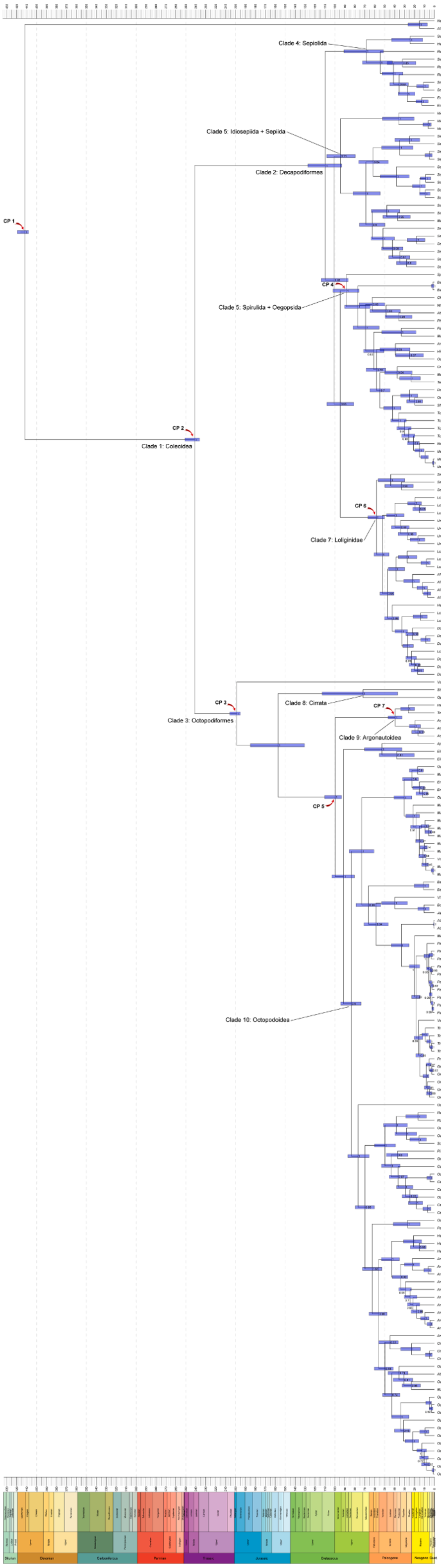

Fig. 2. Molecular divergence times of cephalopods. Bars in each node represent 95% High Posterior Density (HPD) intervals on each estimate. CP 1–6 are the calibration points. See Methods for details.

The BAMM analysis based on the MCCT corroborate previous results. BAMM shows an overall increase in diversification rate over coleoid

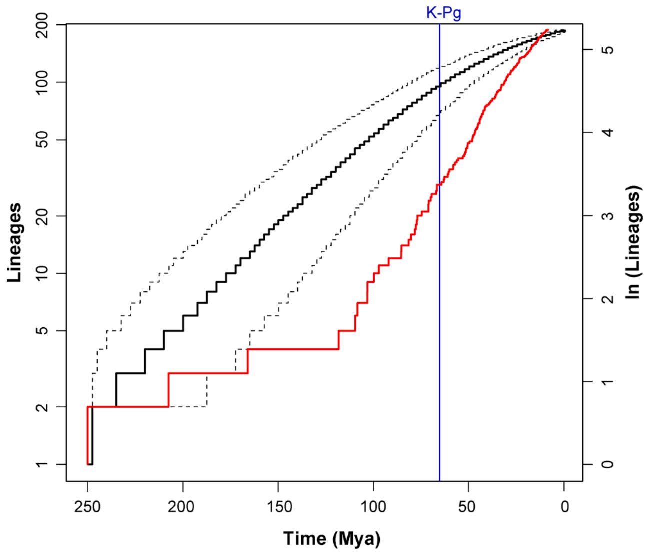

Fig. 3. Comparison plot between observed Lineages Though Time (LTT) for cephalopods and 10,000 simulated LTTs under a pure-birth process. Simulated trees were generated to have a species richness (840 taxa) equivalent to the presumed diversity of coleoid cephalopods, and then pruned randomly to the taxon sampling of this study. Black line represents the mean, and dashed lines are the CI for the LTT from the simulation under a pure birth process. Red line represents the LTT based on the MCCT tree. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

radiation (Fig. 4a). Furthermore, diversification models with discrete shifts in rate are strongly favoured over the null model of no discrete shifts (Bayes Factor > 100). BAMM found that two diversification models are equally likely to describe the diversification pattern of coleoids. Both models reach the highest *posterior* probability, representing the 33% of all the sampled models (17% plus 16% of the *posterior* sample of models, Fig. 4b and c). These models show three discrete shifts of increase in diversification rate before the K-Pg and one shift after the K-Pg (Fig. 4b and c). Regarding the shifts before the K-Pg, one was detected on the branch leading to the species *Vampyroteuthis infernalis* (Fig. 4b), and two shifts on the branches leading to the clade of the superorder Decapodiformes and the clade of the suborder Incirata (Fig. 4c). The post K-Pg shift was detected around 30 Mya, in the branch leading to the Antarctic clade, which contains species of the genus *Megaleledone*, *Thaumeledone*, *Graneledone*, *Praealtus*, *Velodona*, and *Pareledone*.

These results were comparable to those obtained from the random sample of 20 phylogenetic trees. All trees show evidence for a discrete shift on the branches leading to the Antarctic clade, after the K-Pg. 15 trees show evidence for shifts on the branches leading to the clade of the superorder Decapodiformes and the clade of the suborder Incirata. From 2345 trees, just 11 trees show evidence for a discrete shift on the branch leading to *V. infernalis*, before the K-Pg. Overall, BAMM results support the increase in coleoid diversification rate after the K-Pg (hypothesis 1) and the abrupt increase in the mid Cenozoic (hypothesis 2). However, BAMM shows that the diversification rate was also increasing before the K-Pg, a pattern that included abrupt shifts in rate.

4. Discussion

4.1. Divergence times

This study dated the divergence of the Coleoidea from the Nautiloidea around the Early Devonian (~412 Mya). We also found relatively ancient divergence dates for the MRCA between Decapodiformes and Octopodiformes (Middle Triassic, ~241 Mya) and the split between Vampyromorpha and Octopoda (Early Jurassic ~ 199 Mya; Table 1); as well as for the MRCA of Decapodiformes (Early Cretaceous ~ 110 Mya). Tanner et al. (2017) found a slightly earlier split between Decapodiformes and Octopodiformes (Late Carboniferous or Permian) based on a phylogeny calibrated with several fossils and outgroups (Bivalvia, Gastropoda and Annelida), in spite of using different molecular clocks and markers. Our estimated divergence times are consistent with the fossil evidence for the existence of incirrate octopods and oegopsid squids during the Cretaceous (Fuchs et al., 2009; Tanabe et al., 2015). The Paleozoic origin of the Coleoidea inferred here has been widely documented in previous research, both based on paleontological evidence and calibrated molecular clocks (Strugnell et al., 2006; Kröger et al., 2011; Tanner et al., 2017, Uribe and Zardoya, 2017). The MRCA for Octopodiformes and Decapodiformes clades showing the highest species richness are within the last 20 to 50 Mya, as previous studies reported for specific families and genera (Ibáñez et al., 2016; Ulloa et al., 2017; Pardo-Gandarillas et al., 2018). Previous studies estimated earlier or more ancient divergence times for cephalopods compared to our study. Uribe and Zardoya (2017) estimated an earlier origin for Coleoidea, although their results could have been influenced by the fact that these authors used only two fossil calibration points and complete mitochondrial genomes, which evolve faster than nuclear genes. Another study (i.e., Strugnell et al., 2006) estimated a much more ancient origin for Coleoidea, using a fossil of *Plesioteuthis* from the Upper Jurassic (151 Mya) to calibrate the divergence between Ommastrephidae and other oegopsid squids. However, subsequent studies such as Fuchs et al. (2007), demonstrated that plesioteuthids belong to the clade Octopodiformes, and are considered an ancestor of modern octopuses. This fact, among others, may be in part related to the conflicting classifications of cephalopod fossils (see Kröger et al., 2011; Neige et al., 2016), which have produced inconsistent divergence time estimates and thus, discordant conclusions regarding cephalopod evolution. Moreover, coleoid fossils are rare and often incomplete (Kröger et al., 2011), which hinders cataloguing them into a given clade.

4.2. Diversification rates

Our study demonstrate that the Coleoidea radiation started during the Middle Triassic. Their diversification rate pattern was variable – showing increasing rates over the Mesozoic and Cenozoic (Fig. 3, Fig. 4a). Furthermore, there were exceptional instances of increase in diversification rate before and after the K-Pg (Fig. 4b and c). The shifts that precede the K-Pg, were detected in the branch leading to *V. infernalis* and on the branches leading to the clade of the superorder Decapodiformes and the clade of the suborder Incirrata. The shift detected after the K-Pg occurred around 30 Mya during the Cenozoic, on the branch leading to the octopus Antarctic clade.

The results from this study support the widely accepted idea suggesting that many marine invertebrates and vertebrates accelerated their diversification process after the K–Pg period, possibly due to the empty habitats left by the groups that disappeared during the K–Pg extinction (Meredith et al., 2011; Sibert and Norris, 2015). However, our findings also suggest ancient events of increased diversification rates of coleoids before the K-Pg boundary. From a structural and functional point of view, coleoids may have been better equipped to deal with the environmental changes that occurred in the Late Mesozoic, prior to the K–Pg mass extinction, compared to the oldest cephalopods with external shells. Their reduced shell, hydrodynamic shape, and stronger mantle made coleoids faster, which constituted an advantage to colonize different habitats (Arkhipkin et al., 2012; Bizikov, 2004, 2008; Doguzhaeva, 2012; Kröger et al., 2011; Mapes et al., 2010; Nishiguchi and Mapes, 2008; Reitner and Engeser, 1982; Sutton et al., 2016; Fuchs et al., 2016, Hanlon et al., 2018). These novel habitats might have imposed stronger selective pressures that triggered the increase in their diversification rates. This increase during the Cretaceous might have also been due to the disappearance of some predators (Iba et al., 2011;

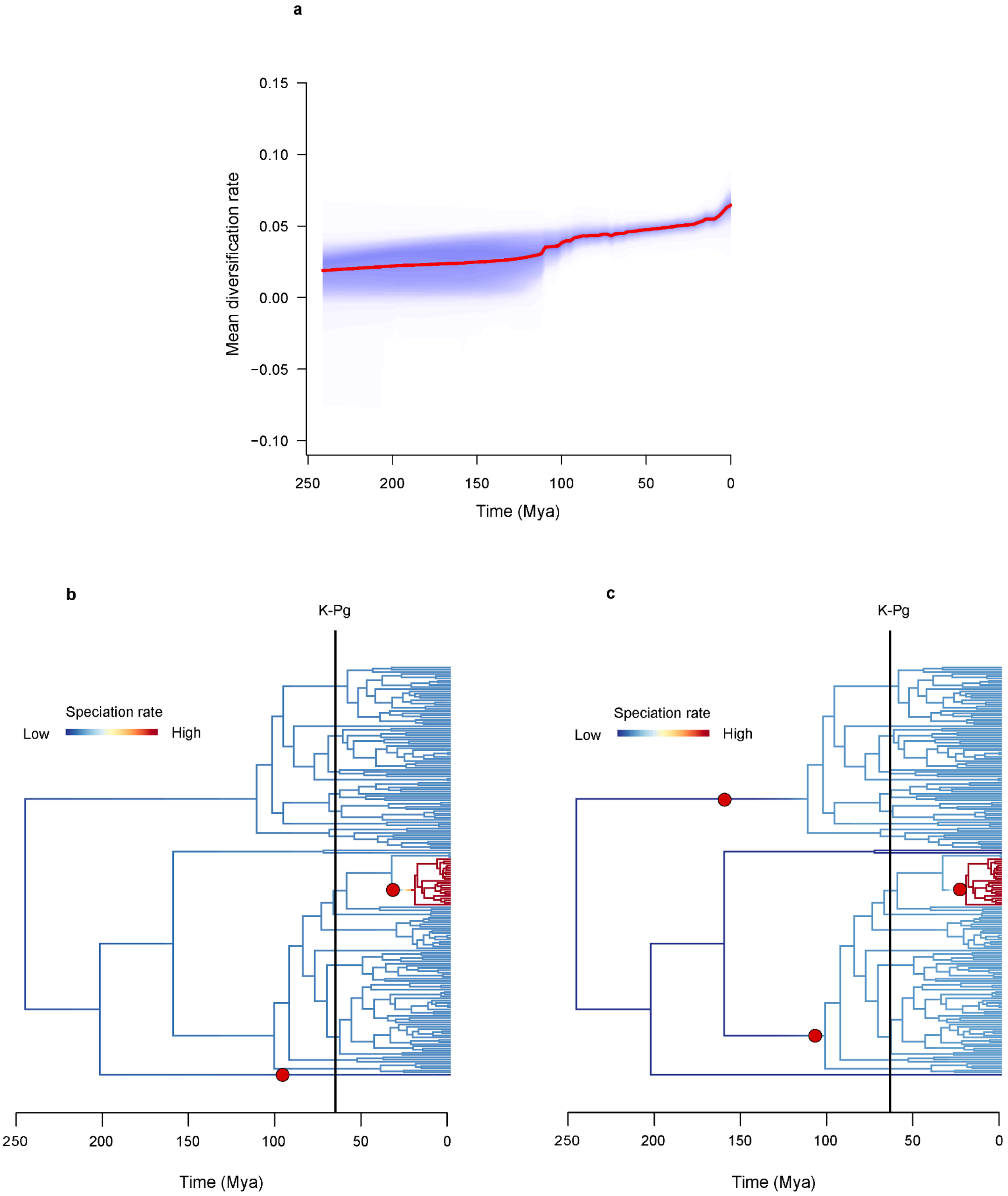

Fig. 4. Diversification rate pattern inferred from BAMM analysis. **a,** the plot shows a pattern of increasing diversification rates over coleoid radiation. The red line shows the averaged diversification rate at any time, estimated from all phylogenetic branches. The shading colour density denotes the confidence on evolutionary rate estimation. **b,** estimated speciation rates across phylogenetic branches given the model with represented in the 17% of the *posterior* probability. **c,** estimated speciation rates across phylogenetic branches given the model represented in the 16% of the *posterior* probability. Branch colours indicate speciation rate values (blue = low, red = high) and red circles on branches indicate the discrete shifts in diversification rate. Vertical black line indicates the K-Pg boundary. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Tanner et al., 2017). For example, the disappearance of the last groups of ichthyosaurs –considered natural predators of coleoids– during the Cenomian-Turonian anoxic event (Lomax, 2010; Molina, 2015; Fisher et al., 2016) could have released coleoids from an ecological constraint, exposing them to strong ecological competition with nektonic marine vertebrates during the Mesozoic (Tanner et al. 2017). On the other hand, during the Mid-Cenozoic, the separation of Antarctica from South America and Australia (Livermore et al. 2005) and the Antarctic ice-sheet formation (Zachos et al. 2001) isolated the Antarctic fauna including some octopus species (Livermore et al. 2005). Furthermore, octopuses evolved toward a holobenthic development (Ibáñez et al. 2014, 2018) and faced the environmental changes associated to the following glaciations, which could promote species range fragmentation and, therefore, could promote the increase in diversification rates observed in the octopus Antarctic clade. This macroevolutionary process may explain the high levels of endemism of benthic octopuses today (Strugnell et al., 2008; Rosa et al., 2019).

Our results support a pattern of increase in diversification rate since the origin of coleoids, associated with the presence of discrete shifts to increase in diversification (Fig. 3, Fig. 4). In any case, it should be noted that our phylogeny represents a low fraction (~20%) of the large diversity of extant cephalopods (~840 species, Hoving et al., 2014), and unsampled species are not missing at random across clades. Currently, some clades (e.g., Myopsida) are sampled much better than others (e.g., Oegopsida, see Table 2). Nonetheless, it is worth mentioning that our methods (e.g. MCCR, LTT) allowed us to minimize the putative estimation errors associated with incomplete taxon sampling, with the caveat that these techniques assume that missing taxa are absent from the phylogeny at random. However, we accounted for the non-randomness of missing species across clades by accounting for the order's sampling fraction in BAMM analyses. Future studies with better sampling of the recognized cephalopod species will improve certainty in macroevolutionary inferences. Above all, our work supports that cephalopod diversity is primarily the result of a rapid diversification of coleoids over time which include exceptional episodes of increased diversification rate before and after the K-Pg boundary.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.ympev.2021.107331.

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