Supplementary material for:

Divergent evolutionary morphology of the axial skeleton as a potential key innovation in modern cetaceans

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Proceedings of the Royal Society B: Biological Sciences

DOI: 10.1098/rspb.2019.1771

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Appendix I: Supplementary methods for *L/H* ratios

Measurements of centrum length and height of 13 fossil specimens were obtained from the literature. Only species that have previously been included in phylogenetic analyses were selected. Data were obtained for four stem cetaceans: *Basilosaurus cetoides* [1], *Dorudon atrox* [2], *Zygorhiza kochii* [1] and *Cythiacetus peruvianus* [3]. Two extinct mysticetes were also included: *Aetiocetus cotylalveus* [4] and *Thinocetus arthritis* [5]. Data were also obtained for seven extinct odontocetes: *Zarhachis flagellator* [6], *Ninoziphius platyrostris* [7], *Kentriodon pernix* [8], *Pliopontos littoralis* [7], *Atocetus iquensis* [9], *Albireo whistleri* [10] and *Piscolithax longirostris* [7]. Measurements were taken from data tables available in the original description of the specimens except for *Albireo whistleri*. For this later species, no raw measurements were available but ratios were obtained from pictures of the backbone available in the original publication. Phylogenetic relationships were synthetized from various recently published phylogenies [11–17].

For extant species, *L/H* ratios were calculated for each vertebra of the thoracic, lumbar and caudal regions. The average ratio for the entire backbone was then calculated and used for the analysis. Densities for the violin plot were computed with the R-package *ggplot2* [18]. The number of vertebrae from which measurements were obtained for extinct specimens varied depending on the preservation state of each specimen but it generally consisted of several vertebrae from at least two different regions of the backbone (apart from the cervical region). Some specimens used were reconstructed from a composite of several specimens. Similar to extant species, the mean *L/H* ratio of each extinct species was then calculated and compared to extant species.

Appendix II: Comparative analyses without phylogenetic correction

1. Material and methods

In order to investigate the raw morphological variation across cetaceans, we repeated all the comparative analyses described in the main text without accounting for phylogenetic information. An identical structure was conserved but all phylogenetically informed analyses were replaced by regular statistics.

(a) Vertebral count and body size.

The effect of habitat on the vertebral count was tested using a regular ANOVA with the function *aov* from the R-package *stats* (v.3.5.1) [19]. We then tested whether Delphinidae and Phocoenidae (i.e. oceanic dolphins and porpoises) differ from the other species in their vertebral count and body size by applying a MANOVA with the *manova* function in R. This analysis was repeated to test such a habitat effect within: (i) Delphinidae and Phocoenidae; (ii) all species except Delphinidae and Phocoenidae; (iii) Delphinoidea; and (iv) non-Delphinoidea. The linear relationship between vertebral count and body length was tested for each group by using a generalized least squares regression (GLS analysis) with the *gls* function from the *nlme* package (v. 3.1-131) [20].

(b) Morphospace of vertebrae.

All linear IMRMs were log10-tranformed and were then size-corrected with a generalised least square regression using the function gls (figure S1e). The \log_{10} TCL was used as a proxy for body size for size-correction. Angular IMRMs (i.e. inclination of neural processes and inclination of transverse processes) were not correlated to body size and were thus transformed using a cosine function. Species mean regional measurements (SMRMs) for linear and angular values were then computed by calculating the mean value of residuals of each IMRM of all individuals belonging to the same species (figure S1e). In order to explore morphological variation of vertebrae, we performed a principal component analysis (PCA) on SMRMs of all cetacean species using the prcomp function in R. PCA was produced on the correlation matrix because the scales of the different morphological traits vary among them. Four distinct PCAs were also run separately for each group: (i) Delphinidae and Phocoenidae; (ii) all species except Delphinidae and Phocoenidae; (iii) Delphinoidea; and (iv) non-Delphinoidea. According to the Jollife cut-off, only principal components (PCs) with an eigenvalue equal to or higher than 0.7 were conserved for further analysis. This corresponds to the first eight PCs for each PCA except the 'Delphinoidea' PCA for which the first nine PCs were conserved. Differences in vertebral morphology between the group of dolphins and porpoises and other species were tested by a MANOVA. A second MANOVA was used to test for a difference between Delphinoidea and non-Delphinoidea. We used a multivariate linear regression to test the correlation between vertebral count and vertebral shape (Joliffe cut-off PCs) for each PCA, using the procD.lm in the R-package geomorph (v. 3.0.6) [21]. For all cetaceans and for every group, we tested the effect of habitat on the variation of vertebral morphology using (c) Evolutionary shifts of phenotypic traits and relationships with the rate of diversification.

BAMM and Bayou analyses, allowing the detection of evolutionary shifts, were performed on PCs 1 to 8 from the 'all cetaceans' PCA that was calculated on non-phylogenetically corrected residuals. Parameters for these analyses were the same as those used for phylogenetically corrected data.

Similarly, the ES-Sim analyses, used to detect the correlation between speciation rate and phenotypic traits evolutionary rates, were performed on non-phylogenetically corrected PCs 1 to 8 with 1,000 iterations. When a significant relationship was found between speciation and a trait, a regular linear model based on generalized least squares was applied to determine the slope of the regression using the *gls* function from the R-package *nlme*.

2. Results

(a) Vertebral count and shape in relation to body size and ecology.

Generally speaking, results obtained from non-phylogenetically corrected analyses regarding the relationship between vertebral morphology and body size and ecology were very similar to those obtained with phylogenetic comparative methods. The sole difference was that the correlation between the vertebral count and body size for all cetaceans was significant without the phylogenetic correction (GLS: p = 0.01, $R^2 = 0.09$) while it was not when accounting for the effect of phylogeny (pGLS: p = 0.7). However, the coefficient of determination was very low, reflecting that the linear regression did not fit well these data. Delphinidae and Phocoenidae differ in body size, vertebral count and vertebral shape from the other families (MANOVAs: $p \leq 0.0001$). Similarly, Delphinoidea differ in vertebral shape from non-Delphinoidea (MANOVA on PCs1-8: $p \leq 0.0001$). Projections of the first two PCs for each PCA are in figures S10 to S12 and statistical results are listed in tables S7 and S8.

(b) Evolutionary patterns of phenotypic traits.

When using uncorrected morphological data for phylogenetic information, BAMM found strong support for a shift occurring for the evolutionary rate of PC1 with 72% of simulated trees having one shift. The principal shift sampled in the posteriors was on the branch leading to beaked whales (*Ziphiidae*) (marginal shift probability: 0.50). However, a shift on one of the branches leading to Delphinoidea was still sampled but with a lower marginal shift probability (0.26) (figure S13). Both these shifts are mutually exclusive meaning that they were never sampled together on the same simulated tree.

Bayou also found support for at least one evolutionary shift for PC1 although the effect was weaker than for phylogenetically-corrected data. Three branches with a posterior probability of having a shift greater than 0.12 (*i.e.* 15 times greater than the prior probability of 0.008) were

sampled. The shift on the branch leading to all Delphinidae except the killer whale (*Orcinus orca*) was still sampled (posterior probability = 0.19) but the shift leading to porpoises (*Phocoenidae*) was not detected anymore. Only a shift on the terminal branch of the Dall's porpoise (*Phocoenoides dalli*) was sampled (posterior probability = 0.13). In addition, a shift on the branch supporting river dolphins (*Pontoporia, Inia* and *Lipotes* genera) was also detected (posterior probability = 0.16) (figure S12). Results of both BAMM and Bayou for PC2 to 8 obtained from the 'all cetaceans' PCA on non-phylogenetically corrected residuals are shown in figure S14.

The results of the ES-Sim test were very similar to those obtained on phylogenetically corrected data. PC1 scores were significantly correlated to the diversification rate (p = 0.03, $R^2 = 0.41$, slope \pm $s.e. = 0.13 \pm 0.02$) while scores on PCs 2 to 8 were not (see table S9).

3. Discussion

Running analyses without accounting for the non-independence of species did not change the main results about the effect of body size and ecology on vertebral count and shape. Analyses on evolutionary patterns (BAMM, Bayou and ES-Sim) still found an evolutionary shift on one of the branches leading to Delphinoidea for PC1. However, the signal was weaker than for analyses on phylogenetically size-corrected data. This is undoubtedly due to the overlap of Delphinoidea and non-Delphinoidea on PC1 that weakens the observed morphological difference between the two groups. Moreover, both methods highlighted other shifts that were less frequently sampled with phylogenetically corrected data which probably also tend to reduce the signal for a shift of the branch leading to Delphinoidea. Nonetheless, the multivariate analysis of variance (MANOVA) ran on PCs 1 to 8 still returned a significant difference between these two groups. This demonstrates that the morphological difference between Delphinoidea and non-Delphinoidea is still present but might be less pronounced on PC1 when data are not phylogenetically corrected.

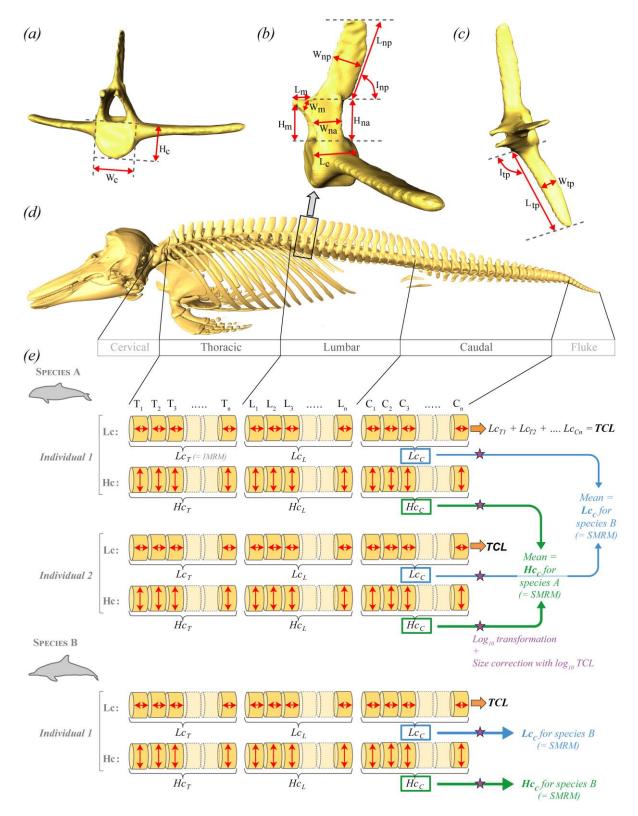


Figure S1. Schematic representation of vertebral shape data collection and standardisation. Twelve linear and two angular measurements (red double arrows) taken on each vertebra are shown on a vertebra in (a) frontal view, (b) lateral view and (c) dorsal view. Wc: centrum width, Hc: centrum height, Lc: centrum length, Lnp: neural spine height, Wnp: neural spine width, Inp: neural spine inclination, Hna: neural arch height, Wna: neural arch width, Lm: metapophysis length, Wm: metapophysis width, Hm: metapophysis height, Ltp: transverse process length, Wtp: transverse process height, Itp: transverse process inclination. (d) 3D model of a harbour porpoise (Phocoena phocoena) skeleton based on CT-scan. Measurements were taken only on vertebrae of three regions: thoracic, lumbar and caudal. (e) For each individual, the mean value of each measurement in each region was calculated (= IMRMs). The total centrum length (TCL) was calculated by summing centra lengths of the three regions. All IMRMs were then log₁₀-transformed and size-corrected using log₁₀ TCL as a proxy for body size. Species values of each measurement of each region (SMRM) were then calculated as the mean of IMRM of all individuals belonging to the species.

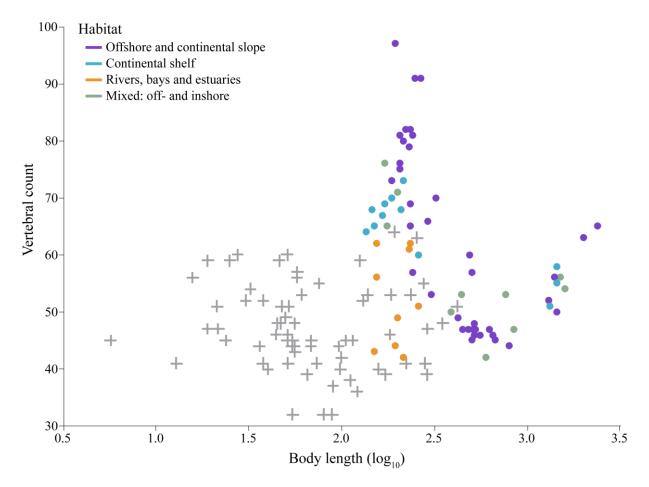


Figure S2. Vertebral counts for cetaceans compared to other mammalian lineages. Vertebral count according to body length in meters (log₁₀-tansformed). Filled circles represent cetaceans; 'plus' signs represent other mammals. For cetaceans, symbol colours correspond to different habitats: orange for rivers, bays and estuaries; light blue for continental shelf; purple for continental slope and offshore; and green for mixed off- and in- shore. For noncetacean species, vertebral count data are from Narita and Kuratani [22] and body size data are from the panTHERIA database [23].

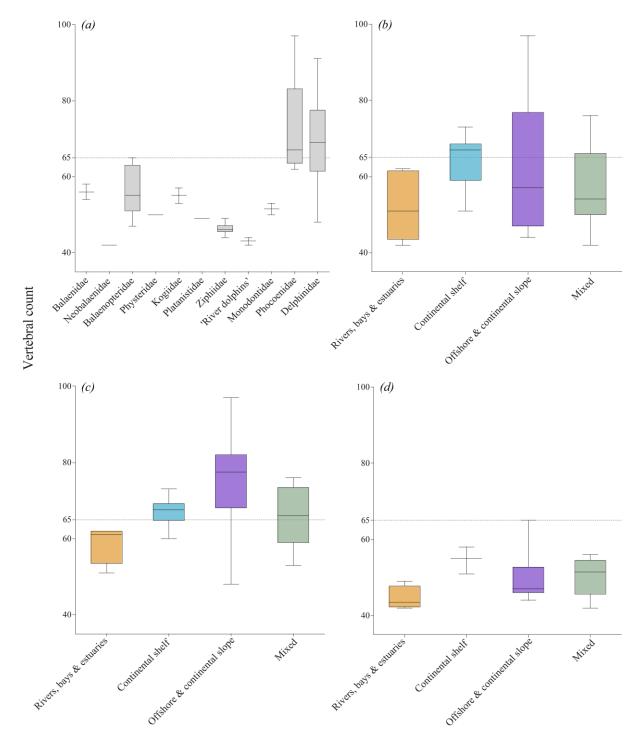


Figure S3. Relationship between vertebral count, family and habitat. Vertebral counts for (a) all cetaceans according to phylogenetic group, (b) all cetaceans according to habitat, (c) Delphinidae and Phocoenidae according to habitat and (d) other cetaceans according to habitat. For each data set, horizontal line represents the median value, lower and upper limits of boxes represent the 25% and 75% quartiles respectively and lower and upper whiskers represent minimum and maximum values respectively.

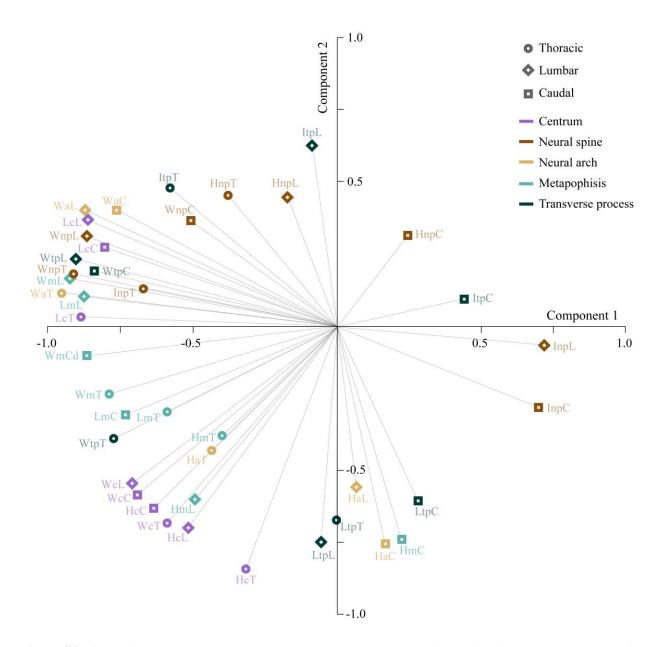


Figure S4. Biplot of the 'all cetaceans' principal components analysis. Loadings of variables on PC1 and PC2 for the PCA calculated on all cetacean species (figure 2). Symbol shapes correspond to the regions of the vertebral column. Each colour corresponds to a different part of the vertebra. Variables abbreviations are explained in figure S1.

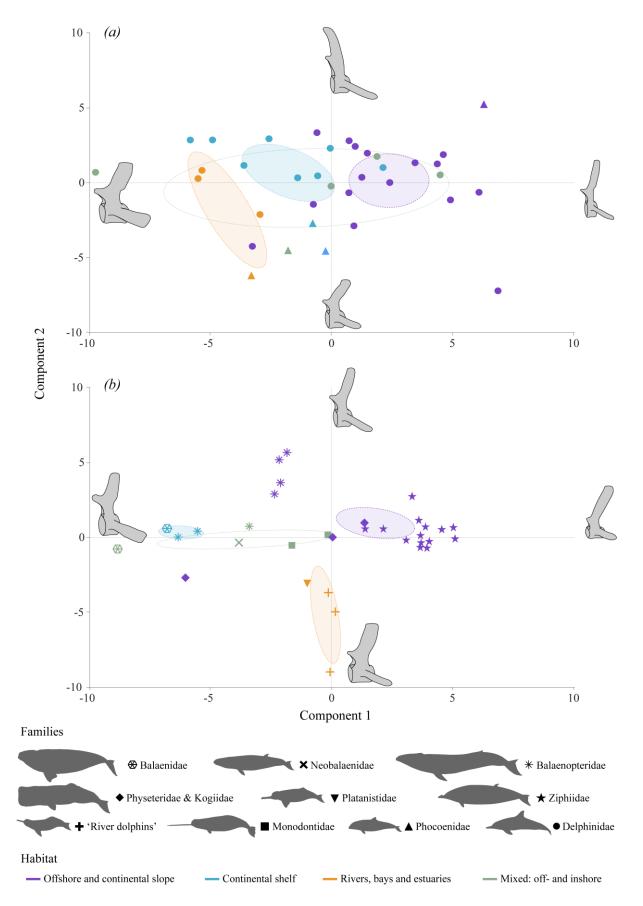


Figure S5. Effect of the habitat on vertebral shape. Principal components analysis plot of PC1 *vs.* PC2. Symbol shapes correspond to phylogenetic groups. Symbol colours correspond to different habitats. Dashed ellipses represent the 95% confidence intervals of the mean coordinates for each habitat category. (*a*) Delphinidae and Phocoenidae. PC1: 35% of variance, PC2: 19%. (*b*) All families excluding Delphinidae and Phocoenidae. PC1: 36%, PC2: 17%.

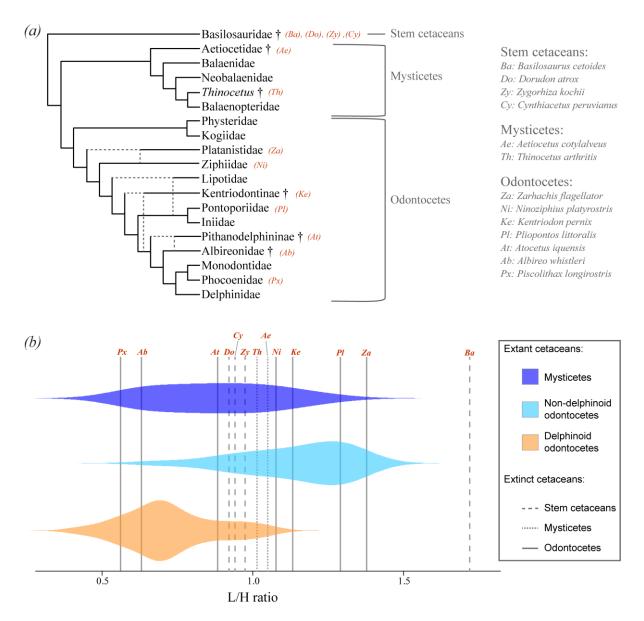


Figure S6. *L/H* ratios of extant and extinct cetaceans. (*a*) Simplified phylogenetic tree of cetaceans including some extinct families and genera (indicated by the dagger symbol) adapted from Marx *et al.* [24]. Dotted lines represent the phylogenetic uncertainty of some lineages. Fossil specimens included in the analysis are annotated in red beside their respective lineage. (b) Violin plot of *L/H* ratios of extant species. *L/H* ratios of extinct species are represented by vertical lines. The name of the species is annotated in red above its corresponding line. Lower ratios correspond to more discoidal vertebrae and higher ratios correspond to more spool-shaped vertebrae.

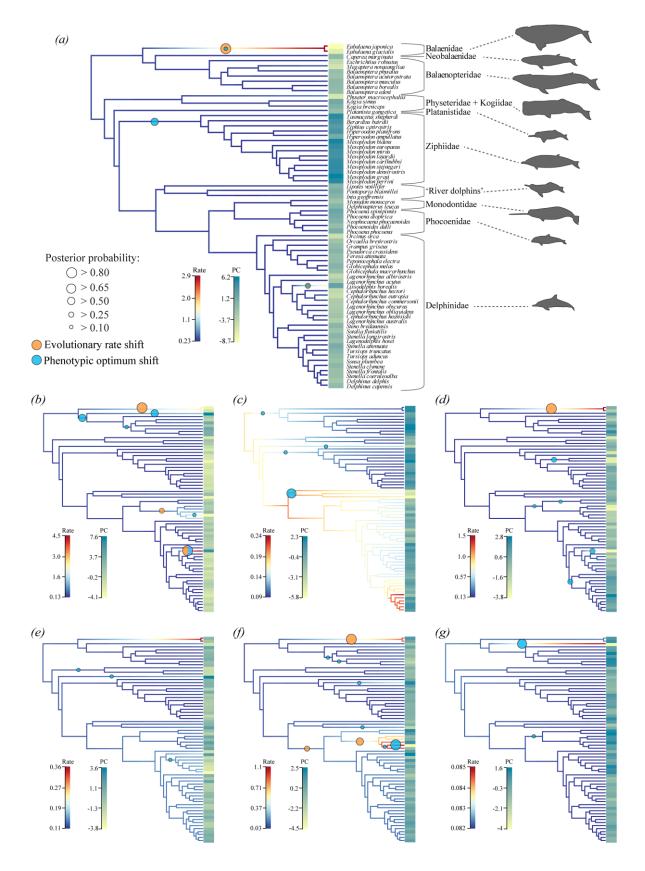


Figure S7. Evolutionary patterns of the vertebral shape (PC2 to PC8). Phylogenetic tree of cetaceans from Steeman [17] with branches coloured according to the evolutionary rates of each principal component from the 'all cetaceans' PCA based on phylogenetically corrected residuals. (a) PC2, (b) PC3, (c) PC4, (d) PC5, (e) PC6, (f) PC7 and (g) PC8. Coloured rectangles at trees tips represent species PC score. Orange circles show shifts in evolutionary rates and were calculated from a Bayesian multi-rate approach (BAMM). Blue circles represent shifts in phenotypic optima and were obtained from a Bayesian multi-regime Ornstein-Uhlenbeck approach (Bayou).

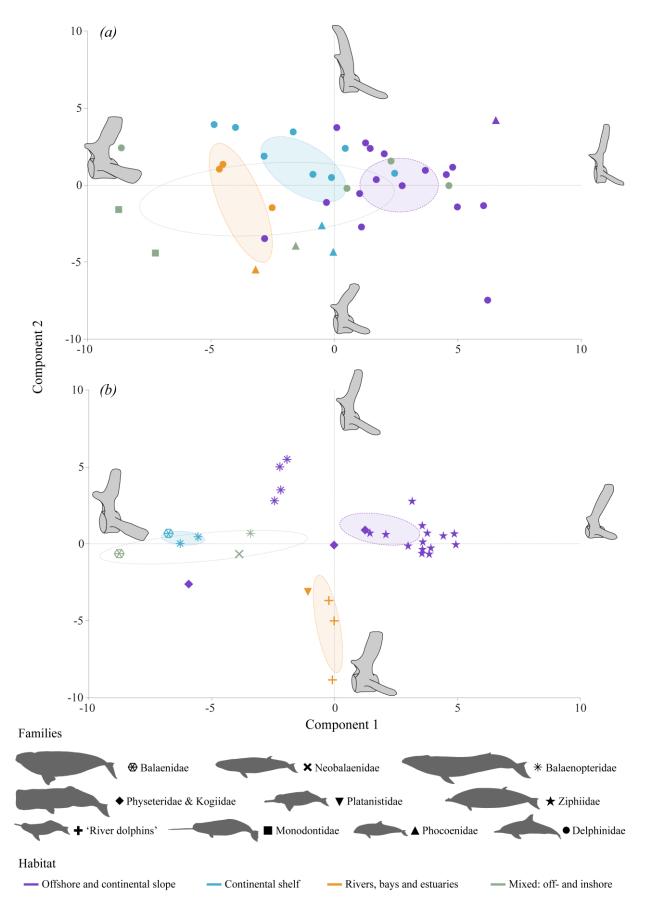


Figure S8. Effect of the habitat on vertebral shape. Principal components analysis plot of PC1 *vs.* PC2. Symbol shapes correspond to phylogenetic groups. Symbol colours correspond to different habitats. Dashed ellipses represent the 95% confidence intervals of the mean coordinates for each habitat category. (*a*) Delphinoidea. PC1: 37% of variance, PC2: 19%. (*b*) Non-Delphinoidea. PC1: 37%, PC2: 18%.

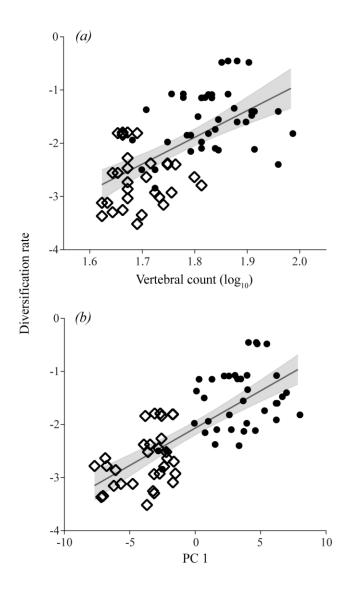


Figure S9. Relationship between diversification rate and phenotypic traits. (*a*) log₁₀-transformed vertebral count. (*b*) PC1 scores from the 'all cetaceans' PCA'. Higher PC1 values correspond to more discoidal vertebrae while lower values correspond to more elongated vertebrae. Filled circles represent Delphinoidea while empty diamonds are for non-Delphinoidea. Diversification rates are the log-transformed speciation rates based on equal splits measure as described by Harvey and Rabosky [47]. For both traits, we found a significant correlation with diversification rates. Solid grey lines represent the linear best fit and grey-shaded areas correspond to the 95% confidence intervals.

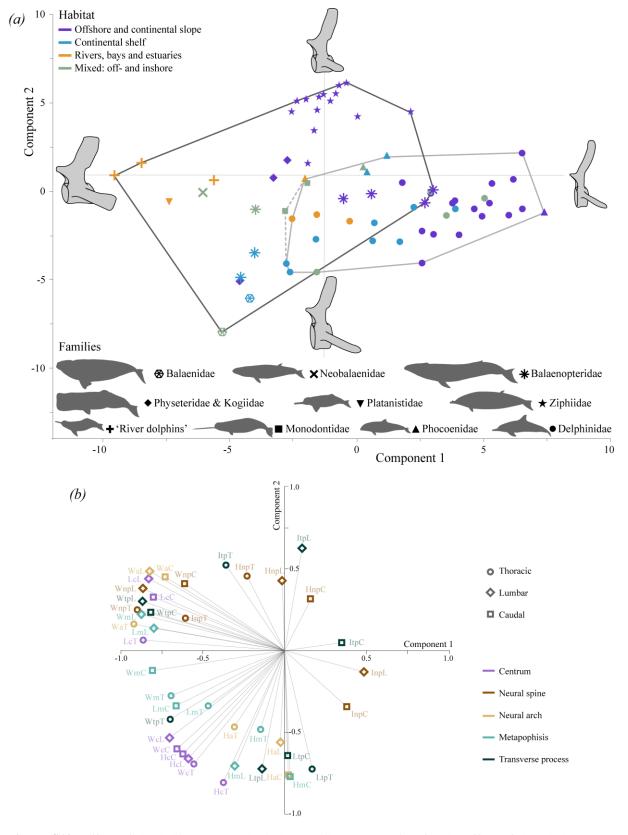


Figure S10. Effect of the habitat on vertebral shape without accounting for the effect of the phylogeny. (a) Projection of species scores on PC1 vs. PC2 for the 'all cetaceans' PCA calculated from non-phylogenetically size-corrected residuals. PC1 represents 35% of the variance and PC2 23%. Typical vertebral shapes are shown at each extremity of the axes. Symbol shapes correspond to phylogenetic groups and colours correspond to habitats. Convex hulls represent (1) Delphinidae and Phocoenidae (grey lines) and (2) non-delphinoidean cetaceans (black lines). Dotted grey lines show the inclusion of Monodontidae with Phocoenidae and Delphinidae. (b) Projection of variable loadings on PC1 and PC2. Symbol shapes correspond to regions of the backbone and colours to different parts of the vertebrae.

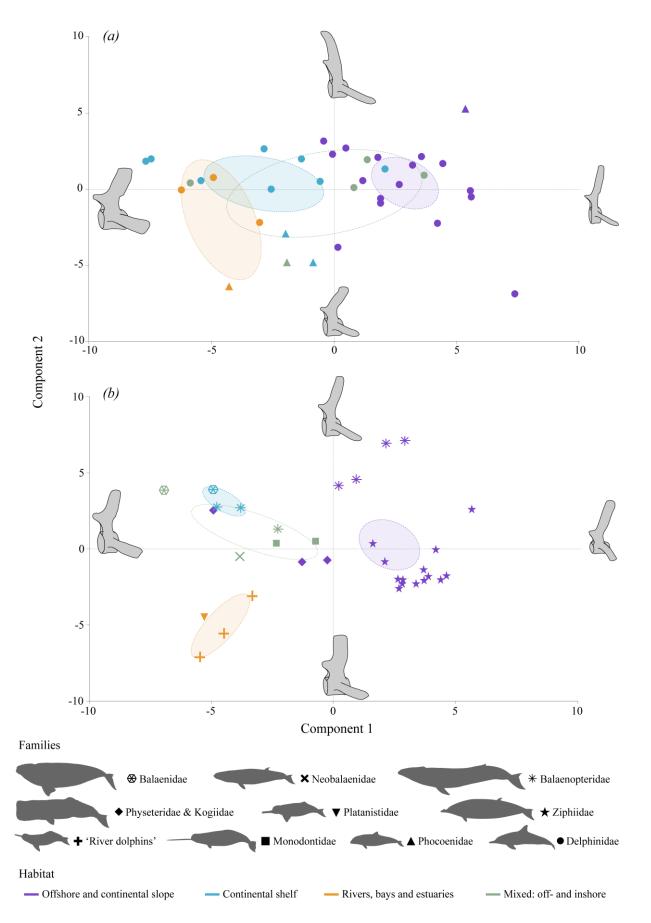


Figure S11. Effect of the habitat on vertebral shape without accounting for the effect of phylogeny. Principal components analysis plot of PC1 *vs.* PC2. Symbol shapes correspond to phylogenetic groups. Symbol colours correspond to different habitats. Dashed ellipses represent the 95% confidence intervals of the mean coordinates for each habitat category. (*a*) Delphinidae and Phocoenidae. PC1: 37% of variance, PC2: 18%. (*b*) All families excluding Delphinidae and Phocoenidae. PC1: 33%, PC2: 27%.

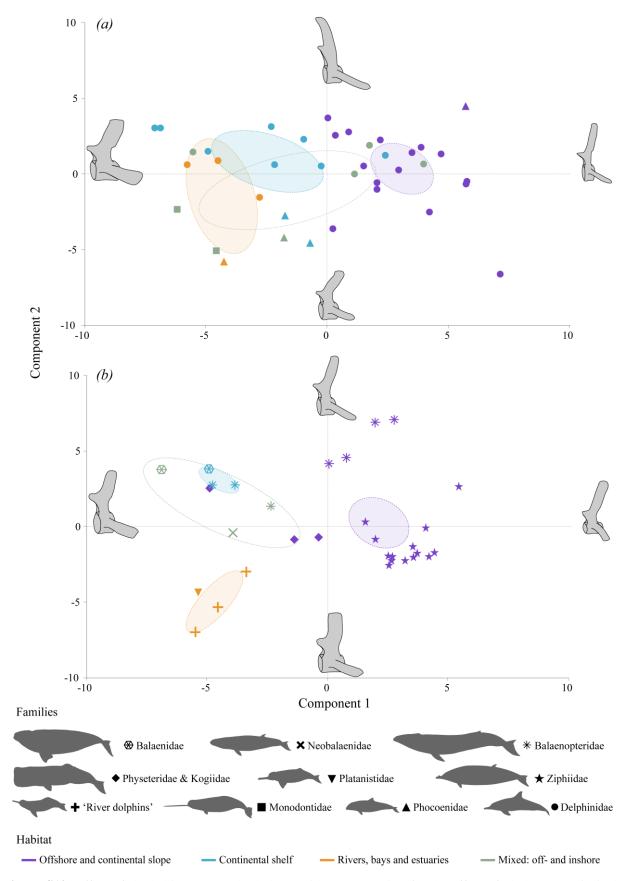


Figure S12. Effect of the habitat on vertebral shape without accounting for the effect of phylogeny. Principal components analysis plot of PC1 *vs.* PC2. Symbol shapes correspond to phylogenetic groups. Symbol colours correspond to different habitats. Dashed ellipses represent the 95% confidence intervals of the mean coordinates for each habitat category. (*a*) Delphinoidea. PC1: 37% of variance, PC2: 18%, (*b*) non-Delphinoidea. PC1: 34%, PC2: 27%.

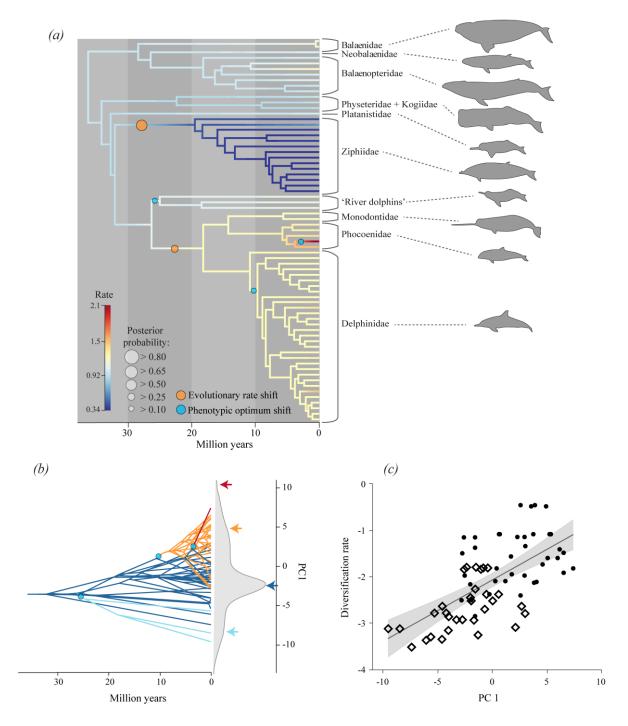


Figure S13. Evolutionary patterns of the vertebral shape (PC1) without phylogenetic correction. (a) Phylogenetic tree of cetaceans from Steeman [17] with branches coloured according to the evolutionary rates of the first principal component (PC1) from the 'all cetaceans' PCA based on non-phylogenetically corrected residuals. Evolutionary rates were obtained from a Bayesian multi-rate approach (BAMM). Grey bands represent 10 million year intervals. (b) Phenogram showing pattern of vertebral shape (PC1) evolution calculated from a Bayesian multi-regime Ornstein-Uhlenbeck approach (Bayou). Phylogenetic tree tips and internal nodes are plotted in function of their vertebral count value. Branches colours show clades with different evolutionary regimes identified by Bayou and coloured arrows correspond to their respective phenotypic optima. Posterior distribution of traits optima is represented by the grey shaded area and their mean value by the coloured arrows. (c) Regression between PC1 and the diversification rate for each species obtained from the ES-Sim test. The solid grey line represents the linear best fit of the statistically significant regression. Grey-shaded area corresponds to the 95% confidence intervals. Orange and blue circles in (a) and (b) show significant shifts of the evolutionary rate (BAMM) and the phenotypic optima (Bayou) respectively. Circles relative sizes correspond to the posterior probability of the shift. Both evolutionary rate shifts identified on (a) are mutually exclusive.

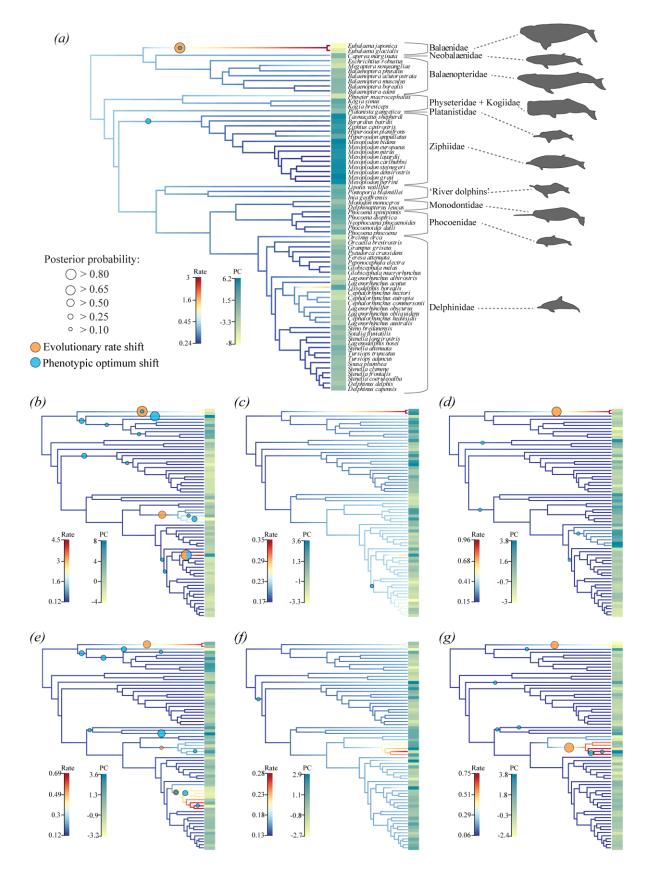


Figure S14. Evolutionary patterns of the vertebral shape (PC2 to PC8) without phylogenetic correction. Phylogenetic tree of cetaceans from Steeman [17] with branches coloured according to the evolutionary rates of each principal component from the 'all cetaceans' PCA based on non-phylogenetically corrected residuals. (a) PC2, (b) PC3, (c) PC4, (d) PC5, (e) PC6, (f) PC7 and (g) PC8. Coloured rectangles at trees tips represent species PC score. Orange circles show shifts in evolutionary rates and were calculated from a Bayesian multi-rate approach (BAMM). Blue circles represent shifts in phenotypic optima and were obtained from a Bayesian multi-regime Ornstein-Uhlenbeck approach (Bayou).

Table S1. List of specimens used in this study. Specimens belong to nine different museums: the American Museum of Natural History, New York (AMNH); the French National Museum of Natural History, Paris (MNHN); the Swedish Royal Museum of Natural History, Stockholm (NRM); the Bayworld Port Elizabeth Museum, Port Elizabeth (PEM); the Queensland Museum, Brisbane (QM); the Royal Belgian Institute of Natural Sciences, Brussels (RBINS); the Iziko South African Museum, Cape Town (SAM); the State Museum of Natural History, Stuttgart (SMNS) and the National Museum of Natural History, Washington D.C. (USNM). For most specimens, both vertebral count and shape data were collected. Specimens on which only vertebral count was collected are marked by a 'C', specimens on which only vertebral shape was collected are marked with an 'S'.

| Balaenidae | | Umana dan planifuana | NDM 559205 |
|----------------------------|--------------------------|--|--------------------------|
| | NDM 550400 C | Hyperoodon planifrons | |
| Balaena mysticetus | NKM 558409 | M 1 1 1 1 1 | SAM ZM41892 |
| Eubalaena australis | | Mesoplodon bidens | |
| Eubalaena glacialis | | | NRM 558398 |
| | NRM 558389 | | USNM 594220 |
| | USNM 593893 | Mesoplodon carlhubbsi | |
| Eubalaena japonica | USNM 339990 ³ | Mesoplodon densirostris | |
| <u>Neobalaenidae</u> | | | USNM 550754 |
| Caperea marginata | RBINS 1536 | | USNM 550951 |
| <u>Balaenopteridae</u> | C. | Mesoplodon europaeus | USNM 550824 |
| Balaenoptera acutorostrata | | | USNM 572952 |
| | USNM 49775 | | USNM 593439 |
| Balaenoptera borealis | | Mesoplodon grayi | |
| | USNM 236680 | Mesoplodon layardii | |
| Balaenoptera edeni | | | SAM ZM19931 |
| | SAM ZM12962 ^s | Mesoplodon mirus | SAM ZM36844 |
| | USNM 572922 | | USNM 504612 |
| Balaenoptera musculus | NRM 558430 ^C | | USNM 504724 |
| | USNM 124326 | Mesoplodon perrini | |
| Balaenoptera physalus | NRM 558431 | Mesoplodon stejnegeri | USNM 504731 ^s |
| | NRM 558434 | | USNM 550113 |
| Eschrichtius robustus | NRM 558391 ^C | Tasmacetus shepherdii | SAM ZM40484 |
| | USNM 593558 ^S | - | USNM 484878 |
| Megaptera novaeangliae | NRM 558433 | Ziphius cavirostris | RBINS 1504 |
| | SAM ZM02288 | • | USNM 347645 |
| Physeteridae | | | USNM 49599 |
| Physeter macrocephalus | NRM 558211 ^s | 'River dolphins' | |
| 1 | NRM 558400 ^C | Inia geoffrensis | MNHN A61 |
| | SMNS 26429 | | SMNS 45662 |
| | USNM 301634 | | USNM 395614 |
| Kogiidae | | | USNM 49582 |
| Kogia breviceps | PEM N1862 | Lipotes vexillifer | |
| | PEM N989 | Pontoporia blainvillei | |
| | SMNS 7618 ^S | | USNM 501168 |
| | USNM 504737 | | USNM 501179 |
| | USNM 572932 | | USNM 504920 |
| Kogia sima | | Monodontidae | 221111 201720 |
| 1108ta sina | PEM N3554 | Delphinapterus leucas | MNHN A3246 S |
| | USNM 504221 | 2 cip.iiiapierus ieneus | NRM 558404 |
| | USNM 593890 | | RBINS 1508 |
| Platanistidae | 221111 273070 | | USNM 571021 |
| Platanista gangetica | MNHN A7945 | Monodon monoceros | MNHN A3235 S |
| 1 ministra gangenea | NRM 608417 ^C | 1.10.10 WOTE THE TOTAL OF THE T | NRM 558407 |
| | SMNS 45652 S | | USNM 594407 |
| | SMNS 45648 | <u>Phocoenidae</u> | CDIMINI DITTOI |
| | SMNS 45651 S | Neophocaena phocaenoides | SMNS 45679 |
| | SMNS 45653 | теорносиени phocuenotaes | SMNS 45680 |
| Ziphiidae | CCOC+ CMINIC | | SMNS 45681 |
| Berardius bairdii | LISNM 40726 S | | USNM 240002 |
| | | Dhagana diartii - | |
| Hyperoodon ampullatus | | Phocoena dioptrica | |
| | RBINS 1503 | | USNM 571486 ^s |

| Phocoena phocoena | NRM 558322 | Lagenorhynchus australis | USNM 395347 |
|-----------------------------|--------------------------|----------------------------|--------------------------|
| | NRM 805026 | | USNM 395350 |
| | NRM 815072 | Lagenorhynchus obliquidens | USNM 504412 ^s |
| | NRM 835011 | | USNM 504413 |
| | NRM 845002 | | USNM 504415 |
| | NRM 855083 | Lagenorhynchus obscurus | SAM ZM41890 ^S |
| | NRM 855196 | | SAM ZM35681 |
| | NRM 865039 ^C | Lissodelphis borealis | USNM 484929 |
| | NRM 865044 | | USNM 550026 |
| | NRM 875045 | Lissodelphis peronii | NRM 558419 ^C |
| | NRM 875216 | Orcaella brevirostris | |
| | NRM 875358 ^C | Orcaella heinsohni | QM JM511 ^C |
| | NRM 895156 | Orcinus orca | MNHN A3231 ^S |
| | NRM 20065226 | | NRM 558250 ^s |
| | RBINS 16233 ^C | | NRM 558251 |
| | USNM 550312 | | NRM 558401 |
| | USNM 571709 | Peponocephala electra | SAM ZM38245 |
| Phocoena spinipinnis | USNM 395751 | | USNM 550399 |
| | USNM 550782 | | USNM 593799 |
| | USNM 550785 ^S | | USNM 593941 ^s |
| Phocoenoides dalli | USNM 396304 | Pseudorca crassidens | NRM 558271 ^S |
| | USNM 504417 | | NRM 558405 |
| | USNM 504969 | | QM J14210 |
| <u>Delphinidae</u> | | | SMNS 7617 |
| Cephalorhynchus commersonii | SAM ZM40555 | Sotalia fluviatilis | RBINS 1516 |
| . , | USNM 550154 | | RBINS 20137 |
| | USNM 550156 | | USNM 571558 |
| Cephalorhynchus eutropia | NRM 616647 | Sousa plumbea | PEM N1179 |
| | USNM 395374 | • | PEM N1266 |
| Cephalorhynchus heavisidii | | | PEM N1582 ^S |
| | SAM ZM19943 | | PEM N1593 |
| | SAM ZM36717 ^S | | USNM 550939 |
| Cephalorhynchus hectori | | Stenella attenuata | USNM 395390 |
| | USNM 500864 | | USNM 396028 |
| Delphinus capensis | | | USNM 500122 |
| | SMNS 45763 ^S | Stenella clymene | USNM 550501 |
| Delphinus delphis | | | USNM 550511 |
| | RBINS 1519B | | USNM 550532 |
| | USNM 500273 | Stenella coeruleoalba | PEM N289 ^S |
| | USNM 593770 | | USNM 504350 |
| Feresa attenuata | PEM N4762 S | | USNM 504384 |
| | PEM N4763 | Stenella frontalis | USNM 21915 |
| | SMNS 8841 | | USNM 22017 |
| | USNM 571268 | | USNM 504321 |
| Globicephala macrorhynchus | USNM 22561 ^S | Stenella longirostris | PEM N1278 S |
| | USNM 593641 | | USNM 395414 |
| Globicephala melas | NRM 558264 | | USNM 500017 |
| _ | USNM 21118 | Steno bredanensis | SAM ZM41124 |
| Grampus griseus | MNHN A3248 | | USNM 504462 |
| | NRM 558392 ^C | | USNM 504468 |
| | PEM N117 S | Tursiops aduncus | SAM ZM38240 |
| | USNM 347613 | - | SMNS 45711 ^S |
| | USNM 504328 | Tursiops truncatus | SAM ZM35678 ^S |
| Lagenodelphis hosei | PEM N395 | | USNM 484529 |
| | PEM N827 ^S | | USNM 504618 |
| | USNM 571619 | | USNM 504726 ^s |
| Lagenorhynchus acutus | USNM 504153 | | USNM 504906 ^s |
| | USNM 504154 | | USNM 550225 |
| | USNM 504164 | | USNM 550364 |
| Lagenorhynchus albirostris | NRM 20065395 | | USNM 550422 |
| _ , | SMNS 7591 | | USNM 550852 |
| | USNM 550208 | | USNM 571388 |
| | | | USNM 572831 |
| | | | |

Table S2. Priors used for the Bayesian multi-regime Ornstein-Uhlenbeck method (Bayou). *1/4 Ntips*: a quarter of the total number of species in the dataset, *Data mean*: mean value of the phenotypic trait of interest for all species, *2 Data SD*: twice the standard deviation of the phenotypic trait of interest for all species.

| Prior | Distribution function | Function parameters | Param. value |
|---------------------------------|-----------------------|-------------------------------------|--------------|
| Constrain parameter (α) | Half-Cauchy | Scale: | 1 |
| Evolutionary rate (σ²) | Half-Cauchy | Scale: | 1 |
| Shift position on branches (sb) | Uniform | Maximum number of shift per branch: | |
| Expected number of shifts (k) | Conditional Poisson | Total number (λ): | |
| | | Maximum number: | 1/4 Ntips |
| Phenotypic optimum (θ) | Normal | Mean: | Data mean |
| | | Standard deviation: | 2 Data SD |

Table S3. Comparison of intra- and interspecific morphological disparity. Interspecific disparity is reported for the entire cetacean clade and intraspecific disparity is reported for two species (*P. phocoena* and *T. truncatus*). The vertebral shape disparity was calculated on size-corrected shape measurements. The absolute disparity of each group is expressed as Procrustes variance in the first part of the table. The second part of the table shows the results of pairwise comparisons of disparity. Significant *p*-values are in bold. *Diff*.: absolute pairwise differences between variances.

| | Vertebral count | | Vertebral shape | | |
|-----------------------------|-----------------|---------|-----------------|---------|--|
| | Variance | | Var | iance | |
| Cetacea | 163.27 | | 0. | 916 | |
| P. phocoena | 18.07 | | 0.293 | | |
| T. truncatus | 4.26 | | 0. | 379 | |
| | Diff. | P-value | Diff. | P-value | |
| Cetacea vs P. phocoena | 145.19 | 0.009 | 0.622 | 0.005 | |
| Cetacea vs T. truncatus | 159.01 | 0.023 | 0.537 | 0.017 | |
| P. phocoena vs T. truncatus | 13.81 | 0.863 | 0.086 | 0.731 | |

Table S4. Summary of correlation tests between body size and vertebral count. The table shows the comparison of the effect of body size on vertebral count when excluding or including Monodontidae with Delphinidae and Phocoenidae. Significant values are indicated in bold.

| Test | | n | P-value | \mathbb{R}^2 | Slope ± s.e. |
|--------------|--|----|---------|----------------|------------------|
| Effect of bo | dy size on vertebral count (PGLS) | | | | |
| | All cetaceans | 71 | 0.7 | -0.35 | -0.27 ± 0.69 |
| | Delphinidae and Phocoenidae | 38 | 0.04 | 0.14 | -4.36 ± 2.00 |
| | Other cetacean families | 33 | 0.0001 | 0.56 | 0.80 ± 0.18 |
| | Delphinoidea | 40 | 0.03 | 0.19 | -4.51 ± 1.93 |
| | Non-Delphinoidea | 31 | 0.0001 | 0.61 | 0.80 ± 0.17 |
| Effect of bo | dy size on vertebral shape (multivariate PGLS) | | | | |
| | All cetaceans | 71 | 0.06 | 0.11 | / |
| | Delphinidae and Phocoenidae | 38 | 0.13 | 0.05 | / |
| | Other cetacean families | 33 | 0.03 | 0.11 | / |
| | Delphinoidea | 40 | 0.07 | 0.06 | / |
| | Non-Delphinoidea | 31 | 0.04 | 0.11 | / |

Table S5. Summary of the effect of habitat on vertebral count and shape. The table shows the comparison of the analysis of variance tests when excluding or including Monodontidae with Delphinidae and Phocoenidae. Significant values are indicated in bold. n: number of species, df: degrees of freedom, F: F-value, P: P-value, P: effect size (eta-squared), ω^2 : effect size (omega-squared).

| Test | | n | df | F | P | η² | ω^2 |
|-----------|-------------------------------------|----|------|------|-------|------|------------|
| Effect of | habitat on vertebral count (pANOVA) | | | | | | |
| | All cetaceans | 71 | 3,67 | 1.87 | 0.39 | 0.08 | 0.04 |
| | Delphinidae and Phocoenidae | 38 | 3,34 | 4.86 | 0.01 | 0.30 | 0.24 |
| | Other cetacean families | 33 | 3,29 | 2.05 | 0.52 | 0.17 | 0.09 |
| | Delphinoidea | 40 | 3,36 | 5.8 | 0.02 | 0.33 | 0.27 |
| | Non-Delphinoidea | 31 | 3,27 | 1.9 | 0.53 | 0.17 | 0.08 |
| Effect of | habitat on vertebral shape (pMANOVA | .) | | | | | |
| | All cetaceans | 69 | 3,65 | 4.96 | 0.001 | 0.35 | / |
| | Delphinidae and Phocoenidae | 36 | 3,32 | 3.03 | 0.001 | 0.46 | / |
| | Other cetacean families | 33 | 3,29 | 6.15 | 0.001 | 0.62 | / |
| | Delphinoidea | 38 | 3,34 | 2.44 | 0.009 | 0.40 | / |
| | Non-Delphinoidea | 31 | 3,27 | 6.99 | 0.001 | 0.62 | 1 |

Table S6. Correlations between diversification rate and morphological traits. The ES-sim test was run with 1,000 iterations on vertebral count and on each principal component (PC) of the PCA applied on all cetacean species. Significant values are indicated in bold. Slope was only calculated for significant correlations.

| Variable | n | <i>P</i> -value | \mathbb{R}^2 | Slope $\pm s.e.$ |
|-----------------|----|-----------------|----------------|------------------|
| Vertebral count | 71 | 0.030 | 0.367 | 5.02 ± 0.79 |
| PC1 | 69 | 0.002 | 0.553 | 0.14 ± 0.02 |
| PC2 | 69 | 0.923 | 0.002 | / |
| PC3 | 69 | 0.675 | 0.033 | / |
| PC4 | 69 | 0.701 | 0.026 | / |
| PC5 | 69 | 0.697 | 0.043 | / |
| PC6 | 69 | 0.777 | 0.019 | / |
| PC7 | 69 | 0.813 | 0.016 | / |
| PC8 | 69 | 0.999 | 0.0001 | / |

Table S7. Summary of correlation tests between body size and vertebral count without phylogenetic correction. The table shows the comparison of the effect of body size on vertebral count when excluding or including Monodontidae with Delphinidae and Phocoenidae. Significant values are indicated in bold.

| Test | | n | P-value | R ² | Slope ± s.e. |
|---|-----------------------------|----|----------|----------------|------------------|
| Correlation between vertebral count and body size (GLS) | | | | | |
| | All cetaceans | 71 | 0.01 | 0.09 | -0.81 ± 0.32 |
| | Delphinidae and Phocoenidae | 38 | 0.01 | 0.15 | -3.47 ± 1.35 |
| | Other cetacean families | 33 | < 0.0001 | 0.57 | 0.75 ± 0.12 |
| | Delphinoidea | 40 | 0.003 | 0.21 | -4.08 ± 1.30 |
| | Non-Delphinoidea | 31 | < 0.0001 | 0.61 | 0.79 ± 0.12 |

Table S8. Summary of the effect of habitat on vertebral count and shape without phylogenetic correction. The table shows the comparison of the analysis of variance tests when excluding or including Monodontidae with Delphinidae and Phocoenidae. Significant values are indicated in bold.

| Test | | n | df | F | P | η² | ω² |
|--------------|-----------------------------------|----|------|------|---------|------|------|
| Effect of ha | bitat on vertebral count (ANOVA) | | | | | | |
| | All cetaceans | 71 | 3,67 | 1.87 | 0.143 | 0.08 | 0.04 |
| | Delphinidae and Phocoenidae | 38 | 3,34 | 4.86 | 0.006 | 0.30 | 0.24 |
| | Other cetacean families | 33 | 3,29 | 2.05 | 0.129 | 0.17 | 0.09 |
| | Delphinoidea | 40 | 3,36 | 5.80 | 0.002 | 0.33 | 0.27 |
| | Non-Delphinoidea | 31 | 3,27 | 1.90 | 0.153 | 0.17 | 0.08 |
| Effect of ha | bitat on vertebral shape (MANOVA) | | | | | | |
| | All cetaceans | 69 | 3,65 | 4.52 | < 0.001 | • | / |
| | Delphinidae and Phocoenidae | 36 | 3,32 | 2.84 | < 0.001 | : | / |
| | Other cetacean families | 33 | 3,29 | 6.15 | < 0.001 | : | / |
| | Delphinoidea | 38 | 3,34 | 2.44 | 0.002 | | / |
| | Non-Delphinoidea | 31 | 3,27 | 6.99 | < 0.001 | | / |

Table S9. Correlations between diversification rate and morphological traits without phylogenetic correction. The ES-sim test was run with 1,000 iterations on each principal component (PC) of the 'all cetaceans' PCA applied on non-phylogenetically corrected residuals. Significant values are indicated in bold. Slope was only calculated for significant correlations.

| Variable | n | P-value | \mathbb{R}^2 | Slope $\pm s.e.$ |
|----------|----|---------|----------------|------------------|
| PC1 | 69 | 0.030 | 0.408 | 0.13 ± 0.02 |
| PC2 | 69 | 0.757 | 0.014 | / |
| PC3 | 69 | 0.470 | 0.085 | / |
| PC4 | 69 | 0.448 | 0.107 | / |
| PC5 | 69 | 0.857 | 0.015 | / |
| PC6 | 69 | 0.685 | 0.042 | / |
| PC7 | 69 | 0.903 | 0.0002 | / |
| PC8 | 69 | 0.929 | 0.001 | / |

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