# Supplement

#### Molecular Data

We used the pipesnakev1.2workflow (Brennan et al. 2024) https://github.com/AusARG/pipesnake to handle, process, assemble, and align our molecular data, estimate gene trees and a species tree. All software employed for individual tasks are indicated in the Supplementary file software versions.yml. Assembled target sequences organized by sample (pseudo-reference genomes; PRGs) are available from XXX. Raw sequence newly sampled taxa are https://data.bioplatforms.com/dataset/?ext\_search\_by=&q=agamidae&organization=ausar g&sequence data type=Illumina+Capture&sort=score+desc%2C+metadata modified+des c&ext bbox=.

# Optima Model Fitting

To explore the reliability of our results concerning the number and species assignment of optima we fit a number of alternative schemes. In addition to the base scheme of PCs 1-6 (>90% variance) and K=0-15, we also fit PCs 1-9 (>95% variance) and all 19 raw trait axes. To assess a more conservative view we also reduced the number of possible shifts, therefore limiting the number of optima to 5 (K=0-4). The results are highly consistent regardless of input data type (PCs vs. raw traits) or trait number (6, 9, 19), in identifying a core set of 4 shifts that are recovered in every scenario. Those correspond to (1) a baseline shift at the base of the Australian radiation of Amphibolurinae, and three shifts that correspond to primarily terrestrial taxa in (2) the edge leading to Moloch, (3) Ctenophorus + Cryptagama, and (4) Tympanocryptis. Additional shifts identified by favored (PCs 1-6) and less conservative (K>4) analyses identify optima that largely correspond to genera, including (5) Lophosaurus, (6) Pogona + Rankinia, (7) Diporiphora, and (8) the large-bodied clade of Ctenophorus. The remaining shifts identify outlying individual species that show unique morphologies, (9) Diporiphora superba, (10) Chlamydosaurus kingii, and (11) Ctenophorus aurita. The final regime belongs to the taxa at the base of the tree comprising Intellagama and Hypsilurus.

Identify breakpoints in increasing hypervolume volume through fitting cubic splines and then comparing the difference in AIC values with increasing number of knots. Biggest jump is going from 2 to 3 knots, which maps to breakpoints at 20 and 10 million years.

# Unsampled Amphibolurinae Taxa

Diporiphora convergens\* STORR, 1974

Hypsilurus binotatus (MEYER, 1874)

Hypsilurus bruijnii (PETERS & DORIA, 1878)

Hypsilurus capreolatus KRAUS & MYERS, 2012

Hypsilurus geelvinkianus (PETERS & DORIA, 1878)

Hypsilurus godeffroyi (PETERS, 1867)

Hypsilurus hikidanus MANTHEY & DENZER, 2006

Hypsilurus longi (MACLEAY, 1877)

Hypsilurus macrolepis PETERS, 1872 Hypsilurus modestus (MEYER, 1874) Hypsilurus nigrigularis (MEYER, 1874) Hypsilurus ornatus MANTHEY & DENZER, 2006 Hypsilurus papuensis (MACLEAY, 1877) Hypsilurus schultzewestrumi (URBAN, 1999) Hypsilurus tenuicephalus MANTHEY & DENZER, 2006 Tympanocryptis uniformis\* MITCHELL, 1948

## Node Priors and Agamids in the Fossil Record

Acrodontan lizards are known from the fossil record of Europe, Australia, and across Asia, with arguably the oldest described lineage originating in Myanmar (Wagner et al. 2021). Unfortunately, the oldest fossil taxa (Protodraco, Gueragama) are of uncertain phylogenetic placement and remaining fossils (Uromastyx europaeus, Barbaturex, Tinosaurus) are considerably younger than recent estimates of subfamily splits in agamids (Title et al. 2024; Burbrink et al. 2020). Agamid fossils are known from Australia (Covacevich 1990; Ramm 2025), however most are comparatively young and unlikely to be of value as calibrations. The exceptions are mid-Miocene agamid fossils from Riversleigh World Heritage Area assigned to Sulcatidens and 'Physignathus'. The latter were ascribed to Physignathus when this genus applied to both P. cocincinus and I. lesueurii, and leaves the current placement of these fossils uncertain. They are clearly Australian in origin, and while similar to *Intellagama*, they also share affinities with *Physiquathus*, *Hypsilurus*, and *Chelosania* (M. Hutchinson, pers. comm.). These fossils were found across a number of Riversleigh sites, all of which have been dated to 16-18 myo by Woodhead et al. (2016): Camel Sputum (17.8), Wayne's Wok (17.8), Inabayance (17.8), Upper (17.8), and RSO (16.6). To use this fossil we applied it as a minimum on the crown of Australian Amphibolurinae, with a soft upper bound of 50 mya informed by estimates of the Amphibolurinae—Draconinae/Agaminae split as estimated by Burbrink et al. (2020) and Title et al. (2024). We applied a secondary calibration on the divergence between Amphibolurinae and Agaminae (*Phrynocephalus*) as a uniform prior with soft bounds (50-80 mya) following Burbrink et al. 2020 and Title et al. 2024, and another uniform prior with soft bounds (238-255 mya) on the crown of Lepidosauria representing the fossil Sophineta, arguably the oldest stem squamate. To assess the appropriateness of this calibration strategy we downsampled our species tree to a single representative of each genus and ran preliminary analyses in MCMCTree.

#### Calculating Morphological Distances

To estimate multivariate morphological distances we calculated euclidean distance between pairs of taxa. For Figure 4 this required identifying transitions among optima and measuring distances between ancestral taxa or between an ancestor and extant taxon (see function node.to.node in script  $XX\_funspace.R$ ).

### Supplementary Figures

Fig.S1 MCMCTree\_PriorPosterior\_NodeLabels. Plots of applied priors (blue), effective priors (pink), and posteriors (green) for each node in the tree indicate reasonable behavior. Node numbers correspond to the phylogeny plotted below, plotted with ape, where n129 is the root node. The effective prior (pink) shows how the interaction of multiple priors can shape the expected ages for a given node. This can be seen when comparing input (blue) and effective

(pink) priors on any calibrated node (e.g. n129, n130, n134).

Fig.S2 Animal\_Measurements. Schematic of morphological measurements taken and outlined in Table S3.

Fig.S3 Amphibolurinae\_CorrPlot. Plot of size-corrected trait correlations with traits grouped by the morphological module they correspond to (either head, body, limb, or tail). Blues indicate positive correlations, red indicate negative correlations, with saturation indicating increasing intensity.

Fig.S4 Amphibolurinae\_Sampling. Locus type and number summarized by sample for newly sequenced samples. Dotted line indicates 50% of targeted sequences recovered. Samples in grey text at left were not included in final analyses.

Fig.S5 Amphibolurinae\_AllLoci\_hASTRAL\_ASTRAL4. Species tree including all samples sequenced and agamid outgroups. Local posterior probabilities are 1 for all nodes except those indicated by an orange circle.

Fig.S6 Amphibolurinae\_Genera\_gCF. Phylogeny of the Amphibolurinae showing intergeneric relationships and support across individual loci. Gene concordance factors (gCF) show the proportion of gene trees which support a given bifurcation. Pie charts on branches indicate the percent of loci which support the presented bifurcation (gCF<sub>1</sub>, orange), one of each of the two other most common resolutions (gCF<sub>2</sub>, blue; gCF<sub>3</sub>, pink) or all other possibilities (gCF<sub>p</sub>, grey). Areas of low concordance (e.g. placement of *Lophosaurus*) indicate topological uncertainty, likely as a result of high levels of incomplete lineage sorting.

Fig.S7 Trait\_Variance. Individual traits show different levels of variance among amphibolurine species, with the greatest variances occurring in size (geometric mean) and tail length. Some traits, such as hand length and upper arm length show vanishingly small variation once corrected for absolute size. (Right) Traits with higher variances are more likely to fit the *fabric* model, which better partitions large changes in trait values.

Fig.S8 VTT\_LTT. The Amphibolurinae hypervolume expands early and late in their evolution, with a period of niche packing in the Miocene. Diversification and morphological expansion are coupled in the early radiation of dragon lizards, but are largely decoupled from the Miocene onwards.

Fig.S9 RF\_PhyloEM\_Optima5. Adaptive peaks corresponding to morphological regimes identified under a multi-optima OU model in *PhyloEM* and applied to ancestral taxa using *randomForests*. (Bottom) Tree shows the preferred 5 regime model estimated from all 19 size corrected morphological traits, with regime shifts denoted by small white circles. (Top) Tree shows the preferred 5 regimes including likelihoods for ancestors as estimated by *randomForest*. The amphibolurine MRCA is estimated as a *Hypsilurus/Lophosaurus*-like arboreal dragon and the Australian MRCA is estimated as a semiarboreal generalist lizard (both indicated with black outline to pie).

Fig.S10 RF\_PhyloEM\_Optima12. Adaptive peaks corresponding to morphological regimes identified under a multi-optima OU model in *PhyloEM* and applied to ancestral taxa using *randomForests*. (Bottom) Tree shows the preferred 12 regime model estimated from the first 6 PC axes of the morphological data, with regime shifts denoted by small white circles. (Top) Tree shows the preferred 12 regimes including likelihoods for ancestors as estimated by *randomForest*. The amphibolurine MRCA is estimated as a *Hypsilurus*-like arboreal dragon and the Australian MRCA is estimated as a semiarboreal lizard (both indicated with black outline to pie).

Fig.S11 HeatMap\_Euclidean\_TreeOrder. Heatmap of multivariate morphological euclidean distance among all pairs of amphibolurines. This presentation highlights the conservative evolution of *Tympanocryptis* along with the relative dissimilarity of novel species like *Chlamydosaurus* (more similar to *Lophosaurus/Hypsilurus*), *Ctenophorus aurita* (more similar to *Tympanocryptis*), and *Moloch*. Black boxes along the diagonal delineate genera or clades of morphologically similar taxa.

Fig.S12 Distance2RegimeCentroid. Multivariate Euclidean distance estimated between each extant species and estimated optima, as well as to the amphibolurine MRCA. Tree at bottom is colored according to the k=5 model of morphological optima. Lollipop plots above show morphological distance between each extant species and the amphibolurine MRCA (black), primarily arboreal regime 1 (red), regime 2 (blue; Tympanocryptis), the primarily generalist regime 3 (yellow), regime 4 (green; Moloch), and regime 5 (orange; Ctenophorus). Based on this metric and our measured traits, the amphibolurine MRCA was most morphologically similar to Intellagama, Physignathus, and Chlamydosaurus. Terrestrial forms like Ctenophorus aurita, the Ctenophorus adelaidensis group, and Tympanocryptis are likely highly derived and morphologically distinct from the MRCA.