

Supplementary data from:

Unique skull network complexity of *Tyrannosaurus rex* among land vertebrates

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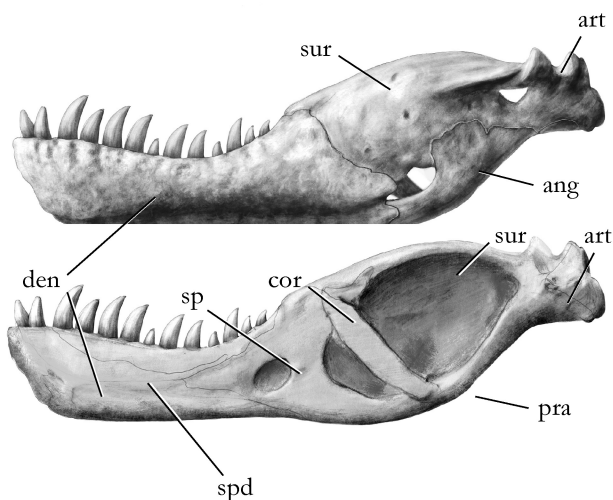
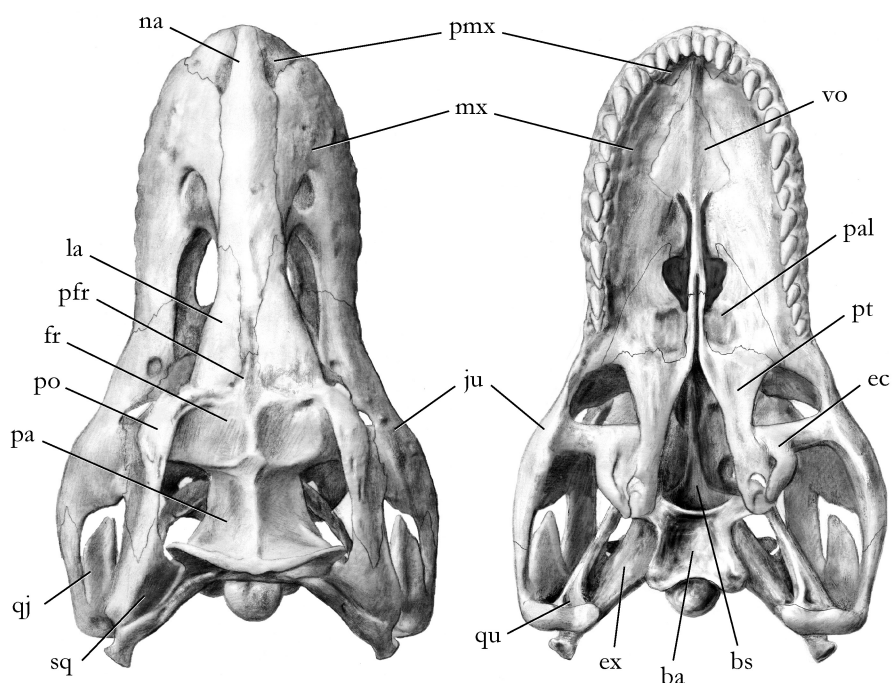
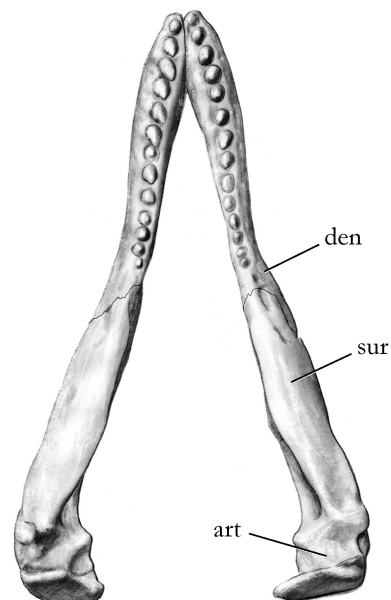
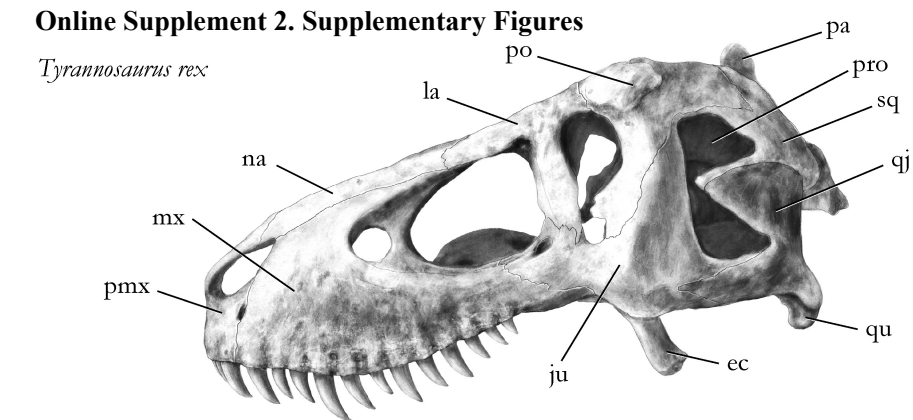


Online Supplement 1. Data Matrices

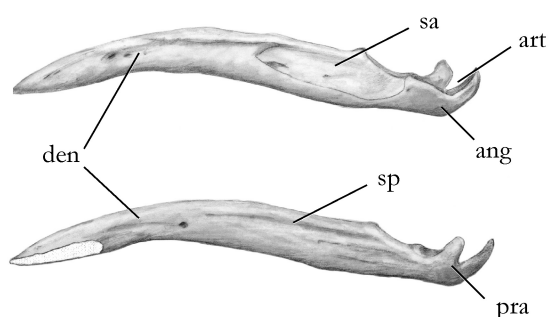
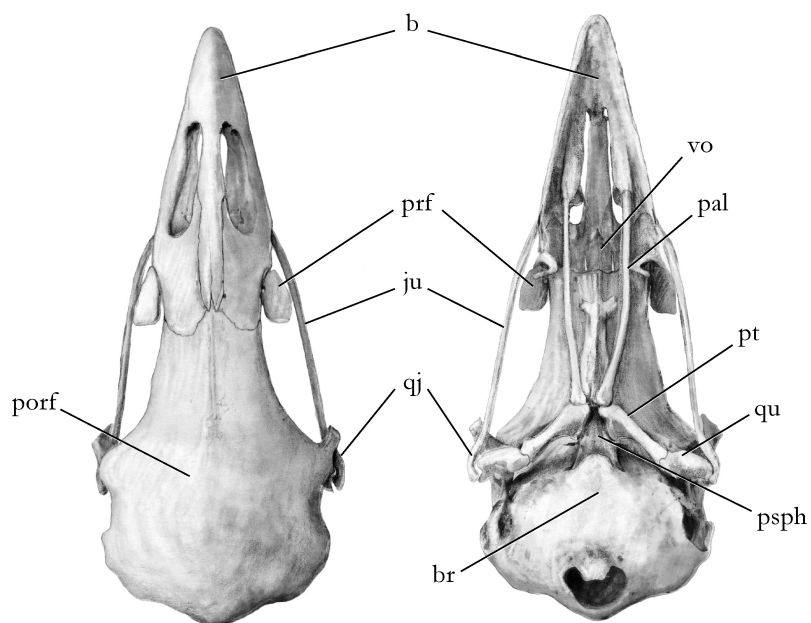
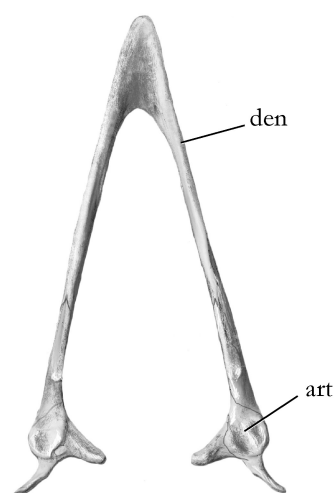
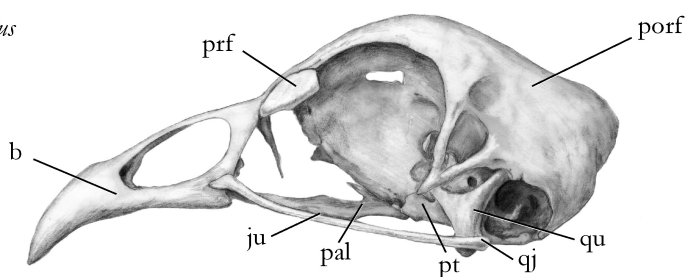
[illegible][illegible]

Online Supplement 2. Supplementary Figures

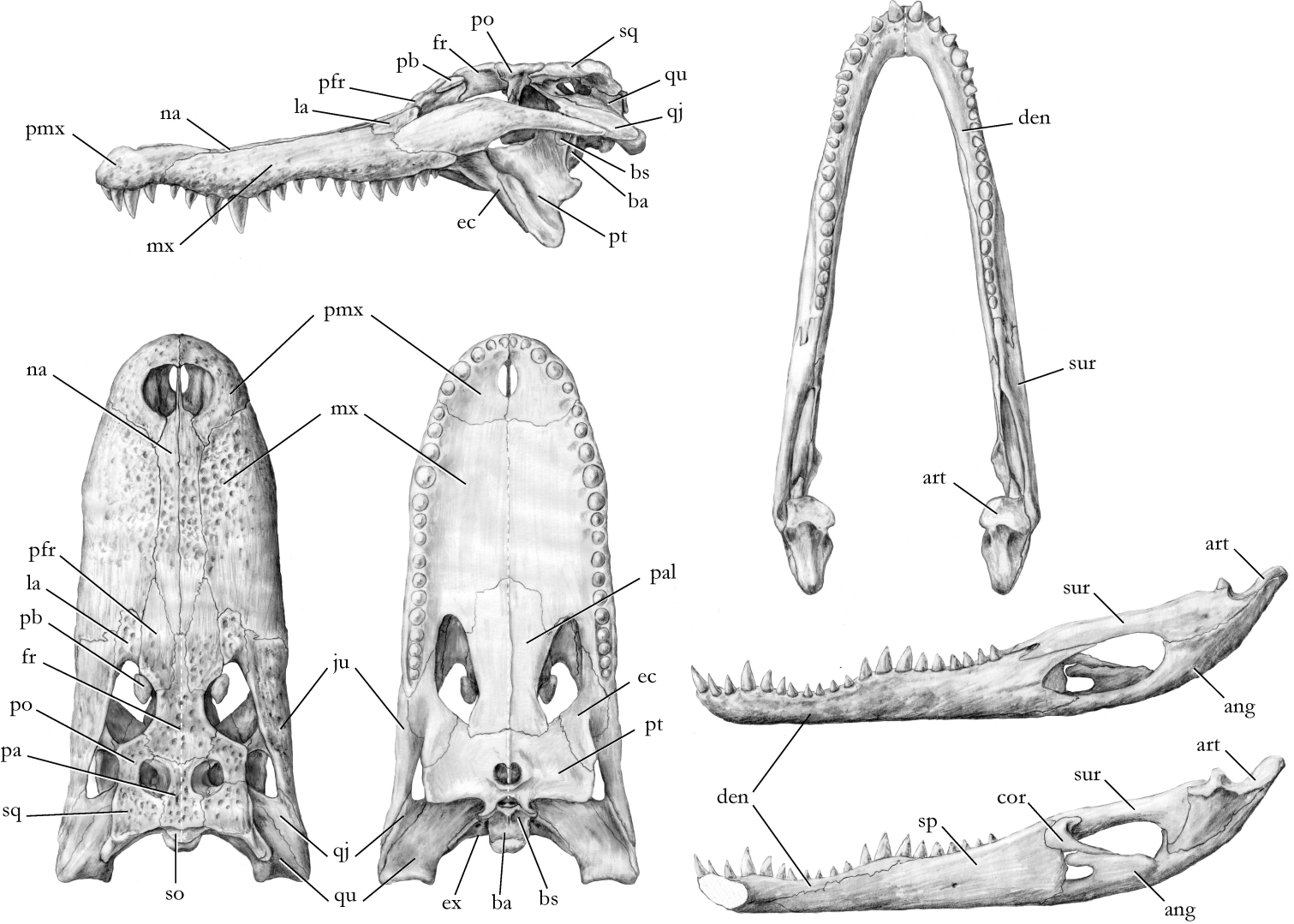
Tyrannosaurus rex



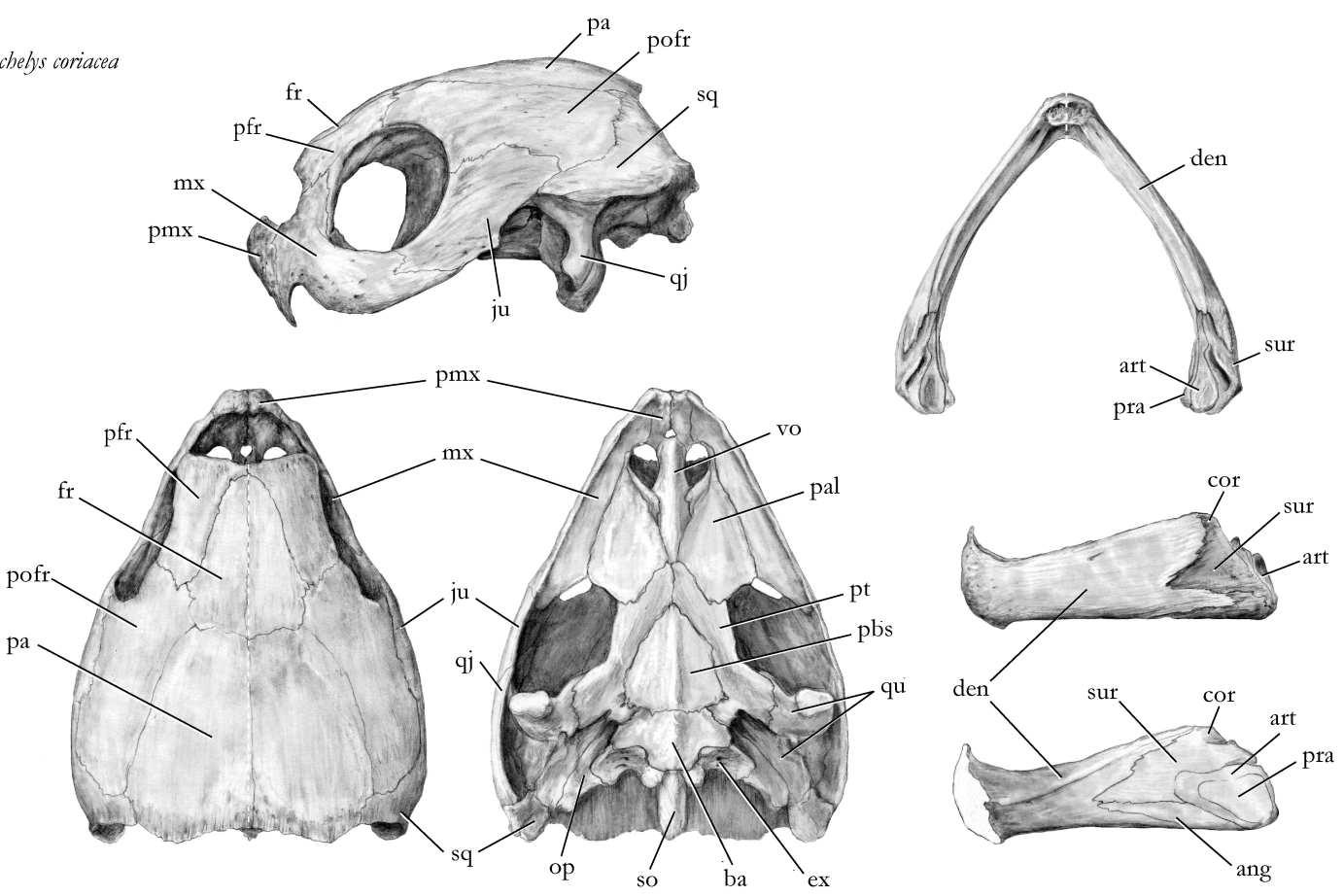
Gallus gallus



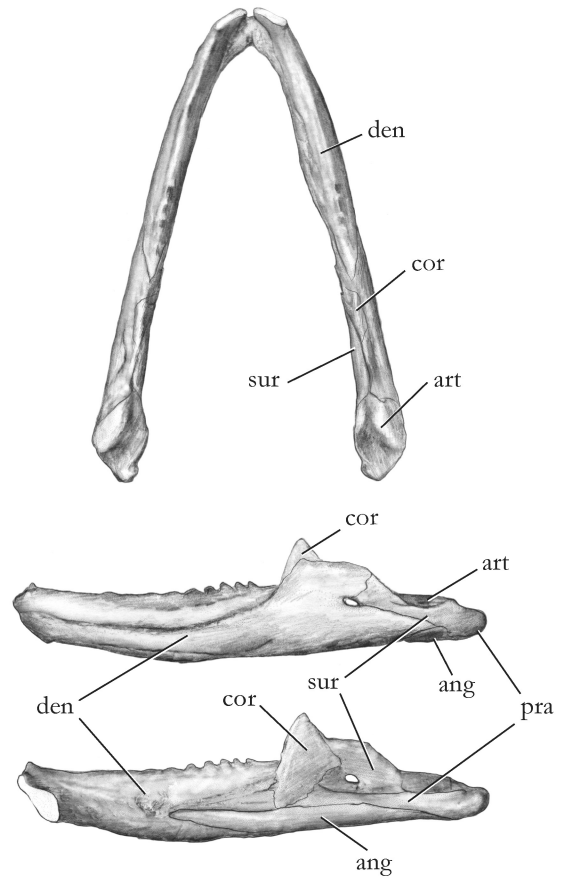
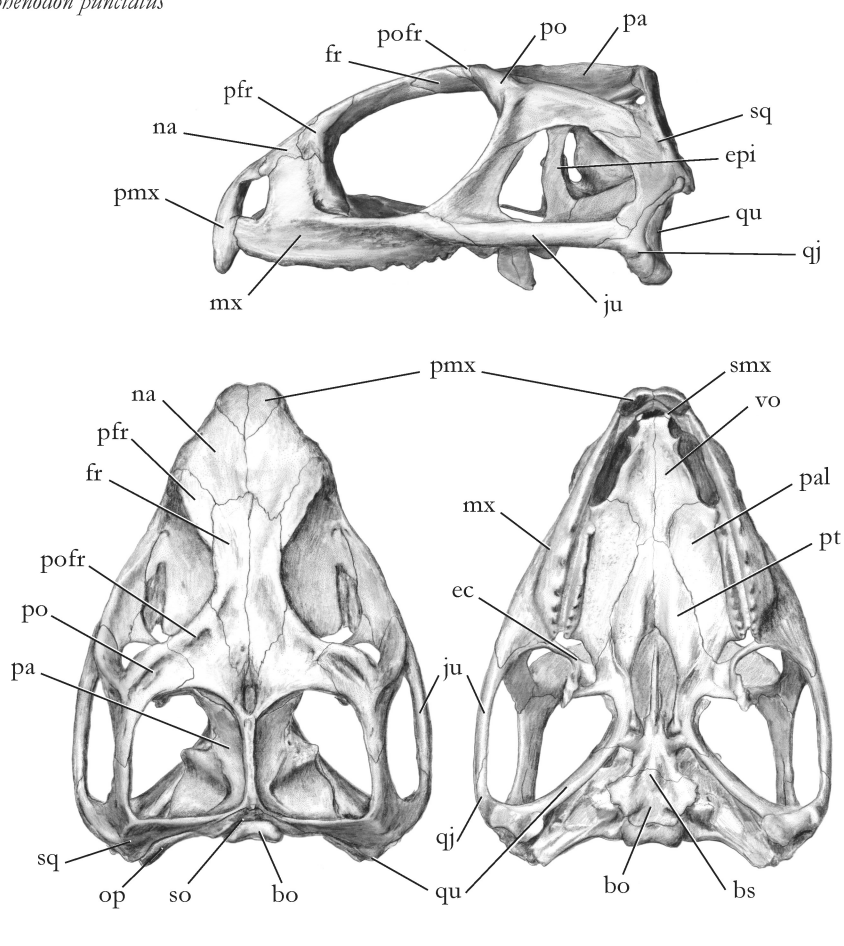
Alligator mississippiensis



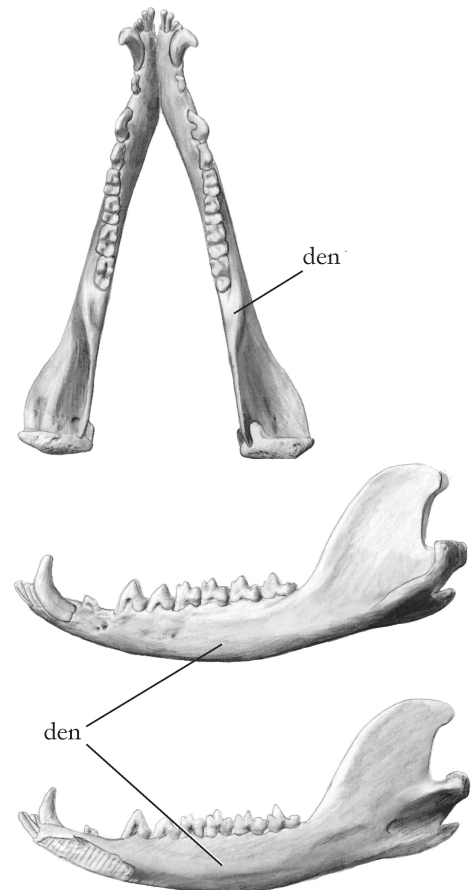
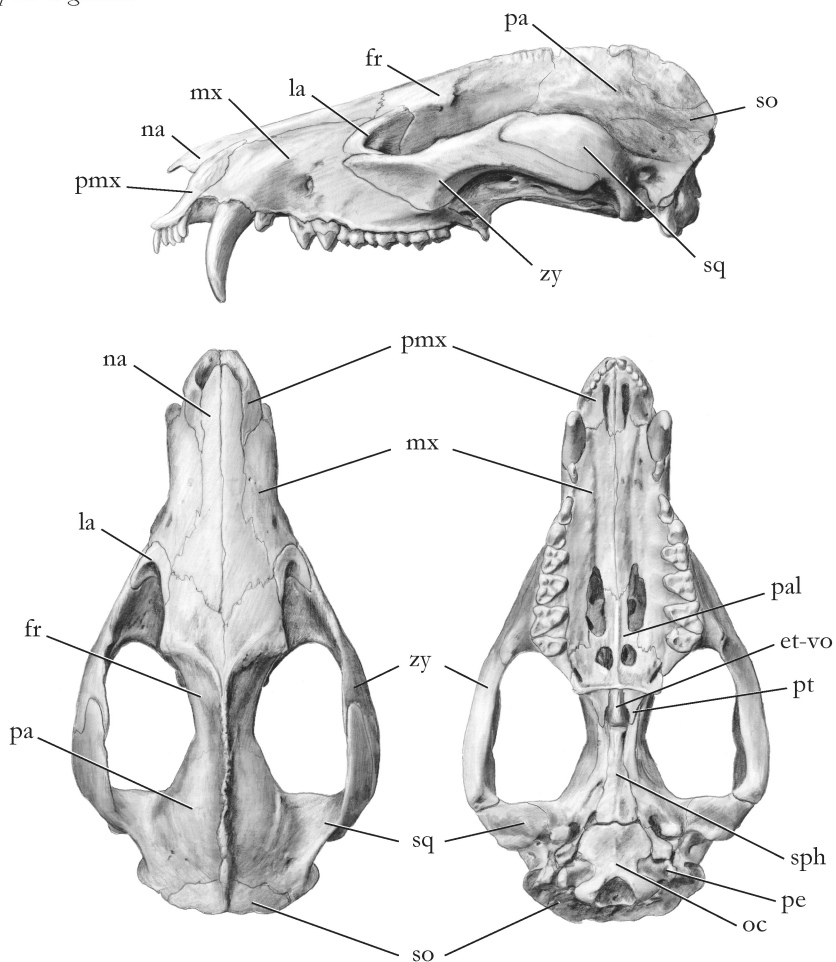
Dermochelys coriacea



Sphenodon punctatus



Didelphis virginiana



Online Supplement 3. R script

```
#####  
#  
#  
# Supplementary Information (R script)  
#  
# Title: Unique skull network complexity of Tyrannosaurus rex among land vertebrates  
# Authors: Ingmar Werneburg et al.  
# Date: 2018  
#  
#####  
##
```

```
# required packages
```

```
library(XLConnect) # load adjacency matrices from Excel to R  
library(igraph) # network analysis  
library(ape) # phylogenetic analysis and hierarchical cluster manipulation  
library(phytools) # phylogenetic analysis and hierarchical cluster manipulation  
library(geiger) # phylogenetic analysis and hierarchical cluster manipulation  
library(adephylo) # phylogenetic analysis and hierarchical cluster manipulation  
library(phylobase) # phylogenetic analysis and hierarchical cluster manipulation  
library(picante) # phylogenetic analysis and hierarchical cluster manipulation
```

```
# load adjacency matrices and create networks
```

```
species <- c("Tyrannosaurus", "Gallus", "Alligator", "Dermochelys", "Sphenodon", "Didelphis")  
mat.list <- mapply(readWorksheetFromFile, "Reptile_Skull_Nets_19Oct2017.xls",  
sheet=1:length(species), rownames=1, check.names=FALSE)  
adj.list <- lapply(mat.list, data.matrix, rownames.force=TRUE)  
pre.graph.list <- lapply(adj.list, graph_from_adjacency_matrix, mode="undirected")  
graph.list <- pre.graph.list  
names(graph.list) <- species
```

```
# generating a file with bone labels
```

```
labels2save <- list()  
for (i in 1:length(species)){  
  num_label <- 1:vcount(graph.list[[i]])  
  names(num_label) <- V(graph.list[[i]])$name  
  labels2save[[i]] <- paste(num_label, names(num_label), sep=" ")  
}  
text.out <- c(species[1], labels2save[[1]], species[2], labels2save[[2]], species[3], labels2save[[3]],  
species[4], labels2save[[4]], species[5], labels2save[[5]], species[6], labels2save[[6]])  
fileConn<-file("Bone Labels Reptiles.txt")  
write(text.out, file=fileConn, ncolums=1)  
close(fileConn)
```

```
## Anatomical Network Analysis
```

```
# parameters
```

```
parameters <- matrix(NA, nrow=length(species), ncol=6) # Table in Figure 1B.  
rownames(parameters) <- species  
colnames(parameters) <- c("N", "K", "D", "C", "L", "H")
```

```

parameters[,1] <- mapply(vcount, graph.list)
parameters[,2] <- mapply(ecount, graph.list)
parameters[,3] <- mapply(edge_density, graph.list)
parameters[,4] <- mapply(transitivity, graph.list, type="average", isolates="NaN")
parameters[,5] <- mapply(mean_distance, graph.list, directed=FALSE)
heterogeneity = function(graph){
  deg = degree(graph)
  res = sd(deg, na.rm=TRUE)/mean(deg, na.rm=FALSE)
}
parameters[,6] <- mapply(heterogeneity, graph.list)

# mapping parameters in the phylogeny (Figure 1C-H)
s <-
"((((Tyrannosaurus:200,Gallus:200):45,Alligator:245):18,Dermochelys:263):21,Sphenodon:284):36,D
idelphis:320);"
cat(s, file = "ex.tre", sep = "\n")
tree <- read.tree("ex.tre")
plotname <- c("Number of nodes (N)", "Number of links (K)", "Density of connections (D)",
"Clustering coefficient (C)", "Shortest path length (L)", "Heterogeneity of connections (H)")
for (i in 1:length(plotname)){
  trait <- as.vector(parameters[,i])
  names(trait) <- species
  fancyTree(tree, type = "phenogram95", x = trait, spread.cost = c(1,0), spread.labels=FALSE,
    xlab = "Time from origin (Myr)", ylab = plotname[i])
  phenogram(tree, x = trait, spread.cost = c(1,0), add = TRUE, ftype = "off")
}

## Community structure (modularity)

# function: GTOM (from http://labs.genetics.ucla.edu/horvath/GTOM/old/gtom.R)
GTOMmdist1 = function(adjmat1,m=1){
  if (m!=round(abs(m))){
    stop("m must be a positive integer", call.=TRUE);}
  if (any(adjmat1!=0 & adjmat1!=1)){
    stop("The adjacency matrix must be binary", call.=TRUE);}
  B <- adjmat1;
  if (m>=2) {
    for (i in 2:m) {
      diag(B) <- diag(B) + 1;
      B = B %%% adjmat1;}} # number of paths with length at most m connecting each pair
  B <- (B>0); # m-step reachability matrix
  diag(B) <- 0; # exclude each node being its own neighbor
  B <- B %%% B; # number of common k-step neighbors that each pair of nodes share
  Nk <- diag(B); # number of common k-step neighbors that each node possesses
  B <- B +adjmat1;
  diag(B) <- 1;
  denomTOM=outer(Nk,Nk,FUN="pmin")+1-adjmat1;
  diag(denomTOM) <- 1;
  1 - B/denomTOM # turn the GTOM matrix into a dissimilarity
}

```

```

# function: prepare adjacency matrices
na.zero <- function(x) {
  x[is.na(x)] <- 0
  return(x)
}

# calculate GTOM and hierarchical clustering
adj.list <- lapply(adj.list, na.zero)
tom.list <- lapply(adj.list, GTOMmdist1, m=1)
dist.tom.list <- lapply(tom.list, as.dist)
hclust.list <- lapply(dist.tom.list, hclust, method="average")
for (i in 1:length(species)){hclust.list[[i]]$labels <- V(graph.list[[i]])$name}
phylo.list <- lapply(hclust.list, as.phylo)

# function: jackknife of modularity Q value
jackknife_Q = function(graph, membership){
  Qi <- vector()
  for (j in 1:ecount(graph)){
    g <- delete_edges(graph, j)
    Qi[j] <- modularity(g, membership)
  }
  ss <- sum((Qi-mean(Qi))^2)
  n <- (ecount(graph)-1)/ecount(graph)
  Q.error <- sqrt(n*ss)
  return(Q.error)
}

# best partition based on Q max
best.partition <- vector()
for (i in 1:length(species)){
  Qvalue <- vector()
  for (j in 1:vcount(graph.list[[i]])){
    Qvalue[j] <- modularity(graph.list[[i]], cutree(hclust.list[[i]], k=j))
  }
  best.partition[i] <- which(Qvalue==max(Qvalue))
}

# function: Wilcox test to evaluate modules
community.significance.test <- function(graph, vids, ...) {
  subgraph <- induced_subgraph(graph, vids)
  indegrees <- degree(subgraph)
  outdegrees <- degree(graph, vids) - indegrees
  wilcox.test(indegrees, outdegrees, alternative="greater")
}

# partition based on statistical significance
Ho_modules_pvalue <- list()
for (i in 1:length(species)){
  graph <- graph.list[[i]]
  tree <- phylo.list[[i]]

```

```

tipN <- vcount(graph)
intN <- tipN-1
Ho_modules_pvalue_v <- vector()
for (j in 1:intN){
  Ho_m <- extract.clade(tree, node=(tipN+j)) # get all subtrees
  is_tip <- Ho_m$edge[,2] <= length(Ho_m$tip.label)
  ordered_tips <- Ho_m$edge[is_tip, 2]
  who <- Ho_m$tip.label[ordered_tips]
  index <- which((V(graph)$name %in% who)==TRUE)
  Ho_mp <- community.significance.test(graph, vids=index)
  Ho_modules_pvalue_v[j] <- Ho_mp$p.value
}
Ho_modules_pvalue[[i]] <- Ho_modules_pvalue_v
}

# dendrogram plots (Figures 2 and 3)
for (i in 1:length(species)){
  plotTree(phylo.list[[i]], lwd=1, mar=c(4.1,1.1,1.1,1.1))
  # p-value groups
  sign <- which(Ho_modules_pvalue[[i]]<0.05)
  bs <- Ho_modules_pvalue[[i]][sign]
  co <- c("black", "grey", "white")
  p <- character(length(sign))
  p[bs < 0.001] <- co[1]
  p[bs >= 0.001 & bs < 0.01] <- co[2]
  p[bs >= 0.01 & bs < 0.05] <- co[3]
  nodelabels(node=(sign+vcount(graph.list[[i]])), pch=21, bg=p, cex=2)
  nodelabels(phylo.list[[i]]$node.label, node=(sign+vcount(graph.list[[i]])), adj=c(1.1,-
0.7),frame="none")
  # Qmax groups
  obj <- ltt(phylo.list[[i]], plot=FALSE)
  k <- best.partition[i]
  h <- mean(obj$times[c(which(obj$ltt==k), which(obj$ltt==(k+1))]))
  lines(rep(h,2), par()$usr[3:4], col="red", lty="dashed")
  title(main=paste("Modularity of the skull network of", species[i]))
}

# groping bones by module
members.list <- list()
for (i in 1:length(species)){
  n <- 2
  p <- 0
  end <- FALSE
  while (end==FALSE){
    members <- cutree(hclust.list[[i]], n)
    for (j in 1:n){p[j] <- community.significance.test(graph.list[[i]], vids=(members==j))$p.value}
    if (all(p<0.05)==TRUE){
      n <- n+1
    } else {
      n <- n-1
      p <- 0
    }
  }
}

```

```

    members <- cutree(hclust.list[[i]], n)
    for (j in 1:n){p[j] <- community.significance.test(graph.list[[i]], vids=(members==j))$p.value}
    end <- TRUE
  }
}
members.list[[i]] <- members
}

# modules information (Figure 1B)
modules <- matrix(NA, nrow=length(species), ncol=4)
rownames(modules) <- species
colnames(modules) <- c("S Modules", "Q Modules", "Qmax", "Qmax error")
for (i in 1:length(species)){
  modules[i,1] <- max(members.list[[i]])
  membership <- cutree(hclust.list[[i]], k=best.partition[i])
  modules[i,2] <- best.partition[i]
  modules[i,3] <- modularity(graph.list[[i]], membership)
  modules[i,4] <- jackknife_Q(graph.list[[i]], membership)
}

```

Online Supplement 4. ex.tre (phylogenetic tree file)

```

((((Tyrannosaurus:200,Gallus:200):45,Alligator:245):18,Dermodochelys:263):
21,Sphenodon:284):36,Didelphis:320);

```