ladder_pH.R

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# function to plot ladder diagram
# pka_list: list of pka values, ideally in order of most acidic to
#           least acidic, but sorted later; default values
#           are for citric acid
# ph_axis: logical; defaults to FALSE but TRUE draws pH axis
# type: the type of ladder diagram; options are "arrow," which is the
#       default, or "strip"
# buffer: logical; defaults to FALSE, but TRUE will add buffer regions
# species: option to enter name of weak acid for main title of plot;
#          defaults to NULL, which supresses main title
# labels: option to enter vector of labels for legend; defaults to
#         NULL, which uses a default legend
# locate: x-axis location of arrow or center of strip; defaults to 2
# overlay: logical; defaults to FALSE, but setting to TRUE allows for
#          adding a new ladder diagram

library(shape)

ladder_pH = function(pka_list = c(3.128, 4.761, 6.396),
                     ph_axis = FALSE,
                     type = "arrow",
                     buffer = FALSE,
                     species = NULL,
                     labels = NULL,
                     locate = 2,
                     overlay = FALSE){

  # initial set-up
  # ensures that the pKa values are in order; creates vector of limits
  # for adding labels; creates counter, n, for the number of alpha
  # values; sets colors for strip version of ladder diagram

  pkas = sort(pka_list)
  limits = c(0, pkas, 14)
  n = length(pkas)
  col.func = colorRampPalette(c("steelblue2", "lightyellow2"))
  colors = col.func(n + 1)

  # creates default set of alpha labels if labels are not provided

  if (is.null(labels) == TRUE) {
    labels = rep(0, n + 1)
    for (i in 1:(n + 1)) {
      num.protons = n - i + 1
      labels[i] = eval(substitute(expression(alpha[I]),
                                  list(I = num.protons)))
    }
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}

# routines for plotting the ladder diagrams for each possible set
# of options: new or overlay; arrow or strip; with or without
# pH axis, and with or without buffer regions

if (overlay == FALSE) {if (ph_axis == FALSE) {
                            phax = "n"
                          } else {
                             phax = "s"
                          }
  plot(NULL, xlim = c(0,14), ylim = c(0,14),
                             type = "n", xaxt = "n", yaxt = phax,
                             bty = "n", xlab = "", ylab = "",
                             xaxs = "i", yaxs = "i")
  }
text(locate + 0.25, 0.5, "pH = 0", pos = 4)
text(locate + 0.25, 13.5, "pH = 14", pos = 4)
if (type == "arrow") {
    Arrows(locate, 0, locate, 14, lwd = 2, arr.type = "simple")
    segments(x0 = rep(locate - 0.3, n), y0 = pkas,
             x1 = rep(locate + 0.3, n), y1 = pkas, lwd = 2)
} else if (type == "strip") {
    for (i in 1:(n + 1)) {
      filledrectangle(mid = c(locate, (limits[i] + limits[i + 1])/2),
                      wx = 0.5, wy = limits[i + 1] - limits[i],
                      col = colors[i], lcol = "black")
    }
} else {
    return(paste(type, " is not an option.", sep = ""))
}
  for (i in 1:n) {
    text(x = locate + 0.25, y = pkas[i],
         labels = paste("pH = ", pkas[i], sep = ""), pos = 4)
  }
  for (i in 1:(n + 1)){
    text(x = locate - 0.25, y = (limits[i + 1] + limits[i])/2,
         labels[i], pos = 2)
  }
  if (buffer == TRUE) {
    if (n == 1) {
      segments(x0 = locate, y0 = pkas - 1, x1 = locate, y1 = pkas + 1,
               lwd = 5, lend = "butt")
    } else { for (i in 1:n) {
      if (i %% 2 == 0){
        segments(x0 = locate + 0.1, y0 = pkas[i] - 1, x1 = locate + 0.1,
                 y1 = pkas[i] + 1, lwd = 5, lend = "butt")
      } else {
        segments(x0 = locate - 0.1, y0 = pkas[i] - 1, x1 = locate - 0.1,
                 y1 = pkas[i] + 1, lwd = 5, lend = "butt")
      }
    }
    }
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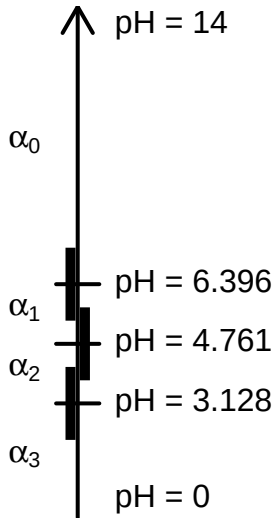
    }
  if (is.null(species) == FALSE) {
    text(x = locate - 1, y = 14, species, pos = 2,
         srt = 90, col = "darkred")
  }
}

# code to test

ladder_pH(type = "arrow", buffer = TRUE)
```

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ladder_pH(type = "strip", buffer = TRUE,
          species = "citric acid", ph_axis = TRUE)
ladder_pH(type = "strip", buffer = TRUE, locate = 7, overlay = TRUE,
           pka_list = c(2.33, 4.42, 9.95), species = "glutamic acid")
```