

ladder_pL.R

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# function to plot ladder diagram for metal-ligand complexes
# pk_list: list of pK values, in order of fewest ligands to most
#         ligands; default values are for cadmium-ammine complexes
# ligands: list giving number of ligands added for each pK value;
#         defaults to vector of (1, 1, 1, 1) for the four stepwise
#         cadmium-ammine complexes
# pL_axis: logical; defaults to FALSE but TRUE draws pLigand axis
# pL_limit: limits for pLigand axis; defaults to 0 to 14
# 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 to add as title for plot;
#         defaults to NULL, which supresses 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,
#         which is practical lower limit; increase in steps of three
#         will separate diagrams; practical upper limit is 12
# overlay: logical; defaults to FALSE, but setting to TRUE allows for
#         adding a new ladder diagram
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library(shape)
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ladder_pL = function(pk_list = c(2.55, 2.01, 1.34, 0.84),
                    ligands = c(1, 1, 1, 1),
                    pL_axis = FALSE,
                    pL_limit = c(0, 14),
                    type = "arrow",
                    shade = "color",
                    buffer = FALSE,
                    species = NULL,
                    labels = NULL,
                    locate = 2,
                    overlay = FALSE){

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

  pks = pk_list/ligands
  n = length(pks)
  limits = c(pL_limit[2], pks, pL_limit[1])
  if (shade == "color") {
    col.func = colorRampPalette(c("lightyellow2", "steelblue2"))
    colors = col.func(n + 1)
  } else {
    col.func = colorRampPalette(c("gray70", "gray30"))
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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)
  labels[1] = expression(alpha[0])
  num.ligands = 0
  for (i in 1:(n)) {
    num.ligands = num.ligands + ligands[i]
    labels[i + 1] = eval(substitute(expression(alpha[I]),
                                     list(I = num.ligands)))
  }
}

# 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 (pL_axis == FALSE) {
  pLax = "n"
  pLlabel = "pLigand"
  pLaxis = ""
} else {
  pLax = "s"
  pLlabel = ""
  pLaxis = "pLigand"
}
plot(NULL, xlim = c(0,14), ylim = c(pL_limit[1],pL_limit[2]),
      type = "n", xaxt = "n", yaxt = pLax,
      bty = "n", xlab = "", ylab = pLaxis,
      xaxs = "i", yaxs = "i")
text(locate + 0.25, pL_limit[2] - (pL_limit[2] - pL_limit[1])/25,
     pLlabel, pos = 4)
}

if (type == "arrow") {
  Arrows(locate, pL_limit[1], locate, pL_limit[2], lwd = 2,
        arr.type = "simple")
  segments(x0 = rep(locate - 0.3, n), y0 = pks,
          x1 = rep(locate + 0.3, n), y1 = pks, 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 = pks[i],

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    labels = pks[i], 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 = pks - 1/ligands, x1 = locate,
      y1 = pks + 1/ligands, lwd = 5, lend = "butt")
  } else { for (i in 1:n) {
    if (i %% 2 == 0){
      segments(x0 = locate + 0.05, y0 = pks[i] - 1/ligands[i],
        x1 = locate + 0.05, y1 = pks[i] + 1/ligands[i],
        lwd = 5, lend = "butt")
    } else {
      segments(x0 = locate - 0.05, y0 = pks[i] - 1/ligands[i],
        x1 = locate - 0.05, y1 = pks[i] + 1/ligands[i],
        lwd = 5, lend = "butt")
    }
  }
}
}
if (is.null(species) == FALSE) {
  text(x = locate - 1, y = pL_limit[2], species, pos = 2,
    srt = 90, col = "darkred")
}
}

# code to test

ladder_pL(pL_axis = TRUE, type = "arrow", species = "cadmium-ammonia",
  locate = 2, pL_limit = c(0, 5))
ladder_pL(type = "arrow", locate = 5, overlay = TRUE,
  pk_list = c(6.87, 2.03), ligands = c(3, 1),
  species = "zinc-ammonia", pL_limit = c(0, 5))
ladder_pL(type = "strip", species = "cadmium-ammonia", locate = 8,
  pL_limit = c(0, 5), shade = "color", buffer = TRUE, overlay = TRUE)
ladder_pL(type = "strip", locate = 11, overlay = TRUE,
  pL_limit = c(0, 5), pk_list = c(6.87, 2.03), ligands = c(3, 1),
  species = "zinc-ammonia", shade = "gray")

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