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#' ---
#' title: 'BacArena - Escherichia coli'
#' author: 'Paulo Freire'
#' date: 'August 6th, 2021'
#' ---

# Load R-packages
library(glpkAPI)
library(BacArena)
library(data.table)
library(sybilSBML)

setwd("/home/paulofreire/CNPEM/RainbowDots/GapSeq/")

# Load reconstructed models
E.coli <- readRDS("E.coli/versions-ecoli/ecoli-DH5alpha.RDS")

# Construct the organism objects for BacArena simulations
E.coli <- Bac(E.coli)

# Construct the arena size 10x10 grid cells
arena1 <- Arena(n = 10, m = 10)

# For each organism, populate randomly 2 grid cells in the Arena as
# 'starter culture'
arena1 <- addOrg(arena1, E.coli, amount = 2)

# add substrates to arena
#arena_subs1 <- addDefaultMed(arena1, E.coli)
arena_subs1 <- fread("E.coli/M9-medium.csv") # same as gapfill medium
arena_subs1[, ex.rxn := paste0("EX_", compounds, "_e0")]
arena1 <- addSubs(arena1, smax = arena_subs1$maxFlux, mediac =
arena_subs1$ex.rxn, unit = "mM", addAnyway = T)

# Simulation for 13 time steps
CF_sim1 <- simEnv(arena1,time=10, sec_obj = "mtf")

# Plot 1 - E.coli
par(mfrow=c(1,2))
plotCurves2(CF_sim1,legendpos = "topleft",
            subs = c("cpd00027_e0","cpd00011_e0"),
            dict = list(cpd00027_e0 = "D-Glucose",
                        cpd00011_e0 = "CO2"))

# Plot 2 - E.coli_WL
par(mfrow=c(1,2))
plotCurves2(CF_sim1,legendpos = "topleft",
            subs = c("cpd00027_e0", "cpd00007_e0"),
            dict = list(cpd00027_e0 = "D-Glucose",
                        cpd00007_e0 = "O2"))
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