PathQuant Tutorial

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## Introduction

This package was writting with the aim to help researchers have options when they have a list of gene known to be linked with a diease and they would like to to metabolomic study but they don't know what kind of metabolic profile they should study.

It can also be used to form hypothesis about gene-phenotype associations and it open doors to knew possible link between genes and metabolites.

This data Set "AssoData" is a data.frame in which each line contains a gene and metabolite associated to each other. The association used are for Shin & al. which constitute a nice exemple to show the accuracy of the method we developped. This is a subset of Shin & al. association data since all the metabolites and genes they found are not all present in the KEGG database

library("PADIGM")  
  
AssoData <- data.frame("gene" = as.vector(c("hsa:4678","hsa:127343","hsa:1579",  
"hsa:1579","hsa:1579","hsa:34","hsa:34","hsa:34","hsa:257","hsa:26227",  
"hsa:117145","hsa:8884","hsa:2646","hsa:2646","hsa:6509", "hsa:9027",  
"hsa:22930","hsa:33","hsa:1373","hsa:1373","hsa:1373","hsa:1373","hsa:54658",  
"hsa:54658","hsa:8801","hsa:51555","hsa:3827","hsa:56606","hsa:56606",  
"hsa:152926","hsa:152926","hsa:152926","hsa:152926","hsa:6999","hsa:2110",  
"hsa:2110","hsa:3818","hsa:56172","hsa:635","hsa:6583","hsa:6583","hsa:6583",  
"hsa:6583","hsa:6583","hsa:6583","hsa:6583","hsa:6583","hsa:6583","hsa:2766",  
"hsa:10786","hsa:4907","hsa:117247","hsa:117247","hsa:6580","hsa:6580","hsa:196",  
"hsa:5723","hsa:1577","hsa:1577","hsa:55063","hsa:55063","hsa:8972","hsa:10",  
"hsa:10","hsa:10","hsa:3620","hsa:26873","hsa:883","hsa:1384","hsa:220963",  
"hsa:220963","hsa:220963","hsa:220963","hsa:220963","hsa:5832","hsa:6319",  
"hsa:6319","hsa:6319","hsa:3992","hsa:3992","hsa:3992","hsa:3992","hsa:3992",  
"hsa:3992","hsa:3992","hsa:6539","hsa:10599","hsa:10599","hsa:10599","hsa:27165",  
"hsa:27165","hsa:5053","hsa:10019","hsa:35","hsa:374569","hsa:3712","hsa:114294",  
"hsa:49855","hsa:23042","hsa:4363","hsa:54988","hsa:115584","hsa:115584",  
"hsa:2806","hsa:9057","hsa:8140","hsa:284111","hsa:284001","hsa:51477",  
"hsa:11136","hsa:6822","hsa:6822","hsa:6822","hsa:875","hsa:5625","hsa:1890")  
), "metabolite" = as.vector(c("C00503","C00503","C13910","C11002","C19615",  
"C05271","C02838","C05275","C00318","C00065","C01942","C00864","C00159",  
"C00041","C02261","C00437","C07326","C01942","C00037","C00300","C00065",  
"C00719","C00500","C00486","C00091","C00318","C00306","C00366","C00135",  
"C00123","C00671","C00183","C02261","C00078","C05275","C02838","C00306",  
"C00158","C00719","C02939","C02636","C00318","C03017","C02571","C05271",  
"C00510","C08283","C09213","C00262","C04295","C00294","C00082","C00078",  
"C00630","C03017","C07481","C00065","C07635","C12525","C07635","C12525",  
"C07326","C16358","C02946","C16359","C00643","C01879","C02043","C00091",  
"C00318","C03017","C02571","C02862","C05271","C00327","C01530","C08322",  
"C08362","C00219","C16527","C06428","C16522","C16300","C16513","C16513",  
"C00719","C11002","C19615","C04295","C05283","C00064","C00079","C00328",  
"C02862","C00152","C02939","C00091","C00630","C16522","C00091","C05629",  
"C06153","C00137","C05607","C00047","C00328","C00158","C03672","C00137",  
"C02427","C04295","C12525","C04555","C00719","C00148","C00299")))  
#getDistanceAsso("hsa01100", AssoData, TRUE,"xslx")  
  
completeGeneDF <- data.frame("gene" = as.vector(c(  
"hsa:249","hsa:4678","hsa:127343","hsa:1579","hsa:1376","hsa:27329","hsa:34",  
"hsa:257","hsa:51179","hsa:26227","hsa:117145","hsa:9970","hsa:2328","hsa:8884",  
"hsa:2646","hsa:6716","hsa:6509","hsa:9027","hsa:130013","hsa:22930","hsa:33",  
"hsa:1373","hsa:54658","hsa:189","hsa:339896","hsa:54716","hsa:7086","hsa:8801",  
"hsa:51555","hsa:56922","hsa:3827","hsa:200931","hsa:56606","hsa:57733",  
"hsa:152926","hsa:6999","hsa:2110","hsa:3818","hsa:56172","hsa:133688",  
"hsa:635","hsa:6583","hsa:2161","hsa:10455","hsa:54898","hsa:2766","hsa:10786",  
"hsa:7916","hsa:6499","hsa:4907","hsa:135293","hsa:117247","hsa:6580","hsa:196",  
"hsa:1644","hsa:5723","hsa:1577","hsa:55063","hsa:6718","hsa:8972","hsa:26",  
"hsa:10","hsa:148","hsa:3620","hsa:6591","hsa:137872","hsa:26873","hsa:883",  
"hsa:1384","hsa:28","hsa:22982","hsa:1109","hsa:220972","hsa:220963","hsa:1559",  
"hsa:1558","hsa:5832","hsa:84795","hsa:6319","hsa:196743","hsa:11234",  
"hsa:3992","hsa:116519","hsa:8882","hsa:6539","hsa:6540","hsa:10599",  
"hsa:27165","hsa:5053","hsa:10019","hsa:35","hsa:144406","hsa:10257",  
"hsa:81537","hsa:399671","hsa:374569","hsa:3712","hsa:11001","hsa:3990",  
"hsa:114294","hsa:49855","hsa:290","hsa:10101","hsa:23042","hsa:4363",  
"hsa:54988","hsa:123876","hsa:115584","hsa:1071","hsa:2806","hsa:9057",  
"hsa:8140","hsa:26001","hsa:284111","hsa:239","hsa:1636","hsa:284001",  
"hsa:9388","hsa:2639","hsa:51477","hsa:11136","hsa:348","hsa:6822","hsa:2524",  
"hsa:79143","hsa:55304","hsa:875","hsa:5625","hsa:1312","hsa:2678","hsa:1890",  
"hsa:410")))  
  
# complete Metabolite from article  
completeMetaboDF <- data.frame("gene" = as.vector(c("C19891","C19670",  
"C19615","C17715", "C17714", "C17337", "C16884","C16537","C16535","C16527",  
"C16526","C16525","C16522","C16513","C16361","C16359","C16358","C16357",  
"C16356","C16353","C15517","C14386","C13910","C13846","C13747","C13637",  
"C12525","C11457","C11332","C11002","C10172","C09908","C09213","C08362",  
"C08322","C08283","C08277","C08262","C07880","C07675","C07635","C07588",  
"C07481","C07480","C07326","C07130","C07086","C06804","C06804","C06429",  
"C06428","C06426","C06424","C06423","C06153","C05984","C05629","C05627",  
"C05607","C05570","C05466","C05465","C05464","C05463","C05283","C05282",  
"C05273","C05122","C04555","C04483","C04295","C04295","C04230","C04148",  
"C04102","C04006","C03882","C03672","C03642","C03626","C03045","C02979",  
"C02946","C02847","C02679","C02678","C02636","C02630","C02571","C02538",  
"C02494","C02483","C02477","C02427","C02350","C02261","C02242","C02180",  
"C02067","C02043","C01947","C01944","C01942","C01921","C01904","C01879",  
"C01796","C01620","C01601","C01595","C01586","C01585","C01571","C01530",  
"C01517","C01468","C01189","C01157","C01152","C01118","C01089","C01004",  
"C00954","C00864","C00847","C00805","C00803","C00791","C00780","C00762",  
"C00755","C00735","C00719","C00712","C00695","C00671","C00670","C00643",  
"C00642","C00630","C00530","C00527","C00503","C00500","C00491","C00486",  
"C00412","C00408","C00407","C00392","C00387","C00385","C00385","C00366",  
"C00328","C00327","C00318","C00306","C00300","C00299","C00296","C00294",  
"C00262","C00258","C00255","C00249","C00233","C00227","C00219","C00216",  
"C00212","C00188","C00187","C00186","C00183","C00180","C00174","C00159",  
"C00158","C00154","C00152","C00149","C00148","C00137","C00136","C00135",  
"C00123","C00116","C00114","C00100","C00097","C00095","C00093","C00091",  
"C00090","C00086","C00082","C00079","C00078","C00077","C00073","C00072",  
"C00065","C00064","C00062","C00049","C00047","C00041","C00037","C00031",  
"C00026","C00025","C00022","C00009","C16513","C16300","C05275","C05270",  
"C03345","C02939","C00510","C00437","C00141","C00032")));

heatmapFunction("hsa01100", AssoData)

permutationFunction("hsa01100", AssoData,  
 completeGeneDF1, completeMetaboDF1, 500, "histograms")

barplotFunction("hsa01100", AssoData, completeMetaboDF, "hsa:1373")