

MetaDAG experiment example

Version beta 0.2

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1 Load data MetaDag experiment

This is an example of an experiment of [metaDag](#) data with results.

Hash: bb261b6e-95c6-3e39-b82b-b68eea80e30b

URL: <https://bioinfo.uib.es/metadag/handleExperiment/0c982fc3-a45f-3645-b0b9-989a0425da6a>

```
library(tidyverse)
library(igraph)
library(ComplexHeatmap)
library(viridis)
library(circlize)
library(plotly)
library(randomcoloR)
library(factoextra)
library(RColorBrewer)
library(kableExtra)
library(igraph)
library(GGally)
```

The screenshot shows the Metadag Tool interface. At the top, there are two tabs: "Metadag Tool" (selected) and "Web Page". Below the tabs, the experiment details are displayed: Experiment id: ff15c187-62e7-37c2-96a7-c824f7eab671, Experiment name: Eukaryotes, Experiment creator: Pere Palmer. On the left, a sidebar menu includes "Home", "Experiment", and "Results". The main content area is titled "Experiment definition" and contains a sub-section "General data". It says: "Here you can select the files containing the calculations made for your experiment." A table lists three items: "MBB" (checked), "mDAG" (checked), and "Results" (checked). To the right of the table is a section titled "similarities" with a checked checkbox. Below the table is a "Select All" button and two circular arrows for sorting. At the bottom, there is a section titled "MetaDAG files" with a note: "Here, you can select what components have to be added to the downloaded data. The amount of options can be variable depending on the experiment and its configurations." At the very bottom of the interface, there are several logos and text: "ACGTCC", "GGCG", "GACCGT", "110101", "1100", "10010111", "UIB", "Universitat de les Illes Balears", and "Departament de Ciències Matemàtiques i Informàtica".

Metadag Tool Experiment id: ff15c187-62e7-37c2-96a7-c824f7eab671
Web Page Experiment name: Eukaryotes
Experiment creator: Pere Palmer

Experiment definition

Give the values needed to perform the desired experiment.

General data

Here you can select the files containing the calculations made for your experiment.

MetaDAG files

Here, you can select what components have to be added to the downloaded data. The amount of options can be variable depending on the experiment and its configurations.

type	format			representation			Select row
	svg	graphml	raw	Essential	Reaction	Compound	
core	<input checked="" type="checkbox"/>						
pan	<input checked="" type="checkbox"/>						
image	<input checked="" type="checkbox"/>						
data	<input checked="" type="checkbox"/>						
mDAG	<input checked="" type="checkbox"/>						
Compound	<input checked="" type="checkbox"/>						
Select column	<input checked="" type="checkbox"/>						

Actions:

Metadag Tool Experiment id: ff15c187-62e7-37c2-96a7-c824f7eab671
Web Page Experiment name: Eukaryotes
Experiment creator: Pere Palmer

Viewing the results

Once an experiment has been calculated it's possible to view the results. To do this, it's necessary to give the experiment unique identifier supplied in the email sent when the experiment was submitted. This unique identifier is also reported in response to the submission.

In the email sent, an url is given to access directly to the experiment results page.
But here, you can also access to the experiment results with the unique identifier.

Enter the experiment identification code *

ff15c187-62e7-37c2-96a7-c824f7eab671

```
experiment=
"result_0c982fc3-a45f-3645-b0b9-989a0425da6a"
path_exp=paste0("data/",experiment,"/data/")
knitr:::kable(data.frame(
  Directory_files_and_folders=dir(path_exp),
  Type=c(rep("Data file",2),
```

```
rep("Directory",3),
rep("Data file",6),
"Directory")))
```

Directory_files_and_folders	Type
Different_MBB.csv	Data file
Different_mDAG.csv	Data file
Global	Directory
Groups	Directory
Individuals	Directory
Report.pdf	Data file
Results.csv	Data file
Similarities_MBB_MSAMethod.csv	Data file
Similarities_MBB_MunkresMethod.csv	Data file
Similarities_mDAG_MSAMethod.csv	Data file
Similarities_mDAG_MunkresMethod.csv	Data file
TaxonomyLevels	Directory

```
MBB=read_csv(paste0(path_exp,"Different_MBB.csv"),
             show_col_types = FALSE)
_mDAG=read_csv(paste0(path_exp,"Different_mDAG.csv"),
               show_col_types = FALSE)
Results=read_csv(paste0(path_exp,"Results.csv"),
                 show_col_types = FALSE)
save(MBB,mDAG,Results,
      file="MBB_mDag_Results.Rdata")
```

1.1 MBB

In this experiment MBB is a table with 5149 rows and 4122 columns.

```
#100
knitr::kable(MBB[1:20,1:10]) %>%
  scroll_box(width = "100%", height = "200px")
```

MBB Id	natural	#pathways	Protists	Fungi	Plants	Animals	Alveolates	Amoebozoa	Annelids
0	0	0	0	0	0	0	0	0	0
0.0	0	0	0	0	0	0	0	0	0
0.0.0	0	0	0	0	0	0	0	0	0
0.0.0.0	1	1	0	0	0	1	0	0	0
0.0.0.0.0	1	1	0	0	0	1	0	0	0
0.0.0.0.0.0	1	1	0	0	0	1	0	0	0
0.0.0.1	1	1	0	0	0	1	0	0	0
0.0.0.2	1	1	0	0	0	1	0	0	0
0.0.1	0	0	0	0	0	0	0	0	0
0.0.1.0	1	1	0	0	0	1	0	0	0
0.0.1.1	1	1	1	0	0	0	0	0	0
0.0.1.1.0	1	1	1	0	0	0	0	0	0
0.0.1.2	1	1	0	0	0	1	0	0	0
0.0.1.3	1	1	0	0	0	1	0	0	0
0.0.1.4	1	1	0	0	0	1	0	0	0
0.0.1.4.0	1	1	0	0	0	1	0	0	0
0.0.1.4.0.0	1	1	0	0	0	1	0	0	0
0.0.1.5	1	1	1	0	0	0	0	0	0
0.0.1.6	1	4	3	0	0	1	0	0	0
0.0.1.6.0	1	3	0	0	3	0	0	0	0

1.2 mDAG

Abstract/unique mDAG's in this experiment

```
dim(mDAG)
[1] 884 5278
#100
kable(mDAG[1:20,1:10]) %>% scroll_box(width = "100%", height = "200px")
```

mDAG Id	#Categories	Animals	Plants	Fungi	Protists	Alveolates	Amoebozoa	Annelids	Arth...
0001	3	1	0	0	0	0	0	0	
0002	2	0	0	1	0	0	0	0	
0003	2	1	0	0	0	0	0	0	
0004	3	1	0	0	0	0	0	0	
0005	3	1	0	0	0	0	0	0	
0006	3	0	1	0	0	0	0	0	
0007	2	0	1	0	0	0	0	0	
0008	3	0	1	0	0	0	0	0	
0009	3	0	1	0	0	0	0	0	
0010	3	1	0	0	0	0	0	0	
0011	3	1	0	0	0	0	0	0	
0012	3	0	0	0	1	0	0	0	
0013	3	1	0	0	0	0	0	0	
0014	3	0	0	0	1	1	0	0	
0015	2	0	0	1	0	0	0	0	
0016	3	0	0	0	1	0	1	0	
0017	3	1	0	0	0	0	0	0	
0018	3	1	0	0	0	0	0	0	
0019	3	1	0	0	0	0	0	0	
0020	3	1	0	0	0	0	0	0	

```
dim(mDAG)
```

```
[1] 884 5278
```

```
names(mDAG)[1:6]
```

```
[1] "mDAG Id"      "#Categories"  "Animals"       "Plants"        "Fungi"
[6] "Protists"
```

```
head(names(mDAG)[7:(dim(mDAG)[2]-1150)])
```

```
[1] "Alveolates"      "Amoebozoa"      "Annelids"
[4] "Arthropods"       "Ascomycetes"     "Basal angiosperms"
```

```
# 28 to 1213 code MBB: 1 if MBB in mDAG 0
```

1.3 Results

Tabular data **Results** for this experiment

```
#100  
#1:20  
kable(Results[1:20,1:10])%>%  
  row_spec(0, angle = 0) %>%  
  scroll_box(width = "300%", height = "1000px")
```

organism	Categories	Groups
aaf	Protists Stramenopiles Pelagophytes	MSA Cluster 3 MUN Cluster 3
aag	Animals Arthropods Insects	MSA Cluster 2 MUN Cluster 2
aalb	Animals Arthropods Insects	MSA Cluster 2 MUN Cluster 2
aali	Animals Arthropods Insects	MSA Cluster 2 MUN Cluster 2
aalt	Fungi Ascomycetes Dothideomycetes	Fungui and Algae MSA Cluster 3 MSA Fungui and Nemat
aam	Animals Vertebrates Birds	Cluster 1
aamp	Animals Vertebrates Mammals	Cluster 1
aang	Animals Vertebrates Fishes	Cluster 1
aara	Animals Arthropods Insects	MSA Cluster 2 MUN Cluster 2
abe	Fungi Ascomycetes Eurotiomycetes	Fungui and Algae MSA Cluster 3 MSA Fungui and Nemat
abp	Fungi Basidiomycetes	Fungui and Algae MSA Cluster 3 MSA Fungui and Nemat
abv	Fungi Basidiomycetes	Fungui and Algae MSA Cluster 3 MSA Fungui and Nemat
acan	Protists Amoebozoa Acanthamoeba	MSA Cluster 3 MUN Cluster 3
acar	Animals Vertebrates Birds	Cluster 1
acep	Animals Arthropods Insects	MSA Cluster 2 MUN Cluster 2
acer	Animals Arthropods Insects	MSA Cluster 2 MUN Cluster 2
achc	Animals Vertebrates Birds	Cluster 1
ache	Fungi Ascomycetes Eurotiomycetes	Fungui and Algae MSA Cluster 3 MSA Fungui and Nemat
achl	Animals Vertebrates Birds	Cluster 1
acoz	Animals Arthropods Insects	MSA Cluster 2 MUN Cluster 2

```
dim(Results)
```

```
[1] 884 3998
```

```
names(Results)[1] # organisms kegg id class representant of mDAG
```

```
[1] "organism"
```

```
names(Results)[2] # taxonomy separate by /
```

```

[1] "Categories"

names(Results) [3] # mDAG_Id

[1] "Groups"

names(Results) [4] # Full name representant

[1] "mDAG_Id"

names(Results) [6:36] # columns 6 to 2726 Variable Reactions name id: This reaction belongs to

[1] "R00710(1.2.1.3)"      "R00710_rev(1.2.1.3)"    "R00711(1.2.1.5)"
[4] "R00711_rev(1.2.1.5)"   "R00755(4.1.1.1)"      "R00746(1.1.1.2)"
[7] "R00746_rev(1.1.1.2)"   "R00754(1.1.1.1)"      "R00754_rev(1.1.1.1)"
[10] "R00014(4.1.1.1)"     "R00014(1.2.4.1)"      "R03270(1.2.4.1)"
[13] "R02569(2.3.1.12)"    "R02569_rev(2.3.1.12)"  "R00703(1.1.1.27)"
[16] "R00703_rev(1.1.1.27)" "R00200(2.7.1.40)"    "R00658(4.2.1.11)"
[19] "R00658_rev(4.2.1.11)" "R01518(5.4.2.11)"    "R01518_rev(5.4.2.11)"
[22] "R01061(1.2.1.12)"    "R01061_rev(1.2.1.12)"  "R01015(5.3.1.1)"
[25] "R01015_rev(5.3.1.1)"  "R01070(4.1.2.13)"    "R01070_rev(4.1.2.13)"
[28] "R04779(2.7.1.11)"    "R04780(3.1.3.11)"    "R02740(5.3.1.9)"
[31] "R02740_rev(5.3.1.9)"

reactions=names(Results) [-c(1:5)]
reverse_reactions=stringr::str_detect(reactions, "rev")
reverse_reactions=table(reverse_reactions)
dimnames(reverse_reactions)$reverse_reactions=c("One direction",
                                              "Reverse reaction")
reverse_reactions

reverse_reactions
  One direction Reverse reaction
 3399                  594

```

2 Graphs

Read graphs in graphml format

2.1 Individuals graph for each organism

Read individual graph for Homo sapiens (Keg id: hsa) at directory(Individuals/hsa)

```
files_hsa=dir(paste0(path_exp,"Individuals/hsa"))
files_hsa

[1] "hsa_mDAG.graphml"          "hsa_mDAG.pdf"           "hsa_mDAG.svg"
[4] "hsa_mDAG_adj.csv"         "hsa_mDAG_biggerDAG.pdf" "hsa_mDAG_biggerDAG.svg"
[7] "hsa_mDAG_nl.csv"          "hsa_mDAG_structure.csv" "hsa_R_adj.csv"
[10] "hsa_R_nl.csv"             "hsa_RC.graphml"          "hsa_RC.pdf"
[13] "hsa_RC.svg"
```

files_Individual_hsa	Description
hsa_mDAG.graphml	graph mDAG graphml format
hsa_mDAG.pdf	csv graph adjacency matrix of mDAG
hsa_mDAG.svg	plot bigger connected component mDAG pdf format
hsa_mDAG_adj.csv	plot bigger connected component mDAG svg format
hsa_mDAG_biggerDAG.pdf	plot essential MBB mDAG pdf format
hsa_mDAG_biggerDAG.svg	plot essential MBB mDAG svg format
hsa_mDAG_nl.csv	csv names labels MBB vertex of mDAG
hsa_mDAG_structure.csv	csv matrix membership of reactions of each MBB of mDAG ordered by decre
hsa_R_adj.csv	csv graph adjacency matrix of RC graph
hsa_R_nl.csv	csv names labels MBB vertex of RC
hsa_RC.graphml	graph RC graphml format
hsa_RC.pdf	plot RC pdf format
hsa_RC.svg	plot RC svg format

```
graph_mDAG=read.graph(
  paste0(path_exp,
  "Individuals/hsa/hsa_mDAG.graphml"),
```

```

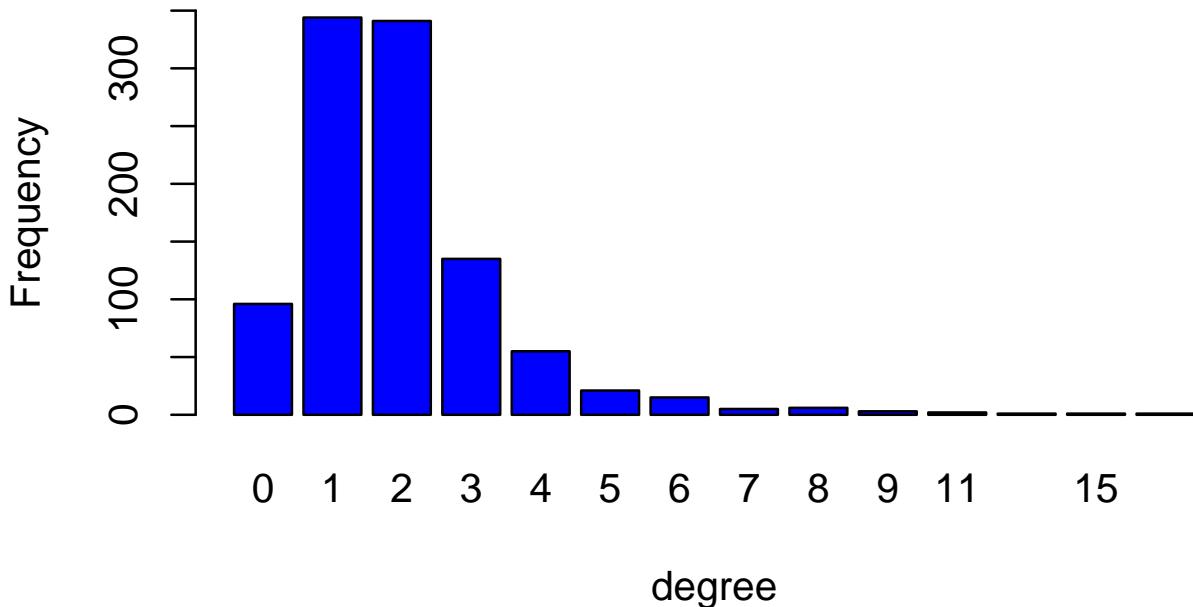
format= "graphml")
summary(graph_mDAG)

IGRAPH 61480b1 D--- 1026 1086 --
+ attr: color (v/c), label (v/c), id (v/c), id (e/c)

barplot(table(igraph::degree(graph_mDAG, mode="all")),
        ylim=c(0,350), col="blue",
        main="Frequency of nodes degree",
        ylab="Frequency", xlab="degree")

```

Frequency of nodes degree



2.2 mDag Global core for eukaryotes

Note that the mDAG core is empty as it does not contain any reactions.

2.2.1 Core mDAG

```

graph_core_mDAG=read.graph(
  paste0(path_exp,"Global/core/core_mDAG.graphml"),

```

```

format = "graphml")
summary(graph_core_mDAG)

IGRAPH 623ebd1 D--- 0 0 --
+ attr: color (v/c), label (v/c), id (v/c)

# file missing
knitr::include_graphics(paste0(path_exp,
                                "Global/core/core_mDAG.pdf"))

```

The graph core mDAG have 0 vertex and 0, is an empty graph.

2.2.2 Core reaction graph (RC)

```

graph_core_RC=read.graph(
  paste0(path_exp,
         "Global/core/core_RC.graphml"),
  format = "graphml")
summary(graph_core_mDAG)

IGRAPH 623ebd1 D--- 0 0 --
+ attr: color (v/c), label (v/c), id (v/c)

knitr::include_graphics(
  paste0(path_exp,"Global/core/core_RC.pdf"))

```

Figure 2.1: Core mDAG is empty

The graph core reaction graph have 0 vertex and 0, is an empty graph.

2.3 mDag Global pan for eukaryotes

2.3.1 Pan mDAG

```
graph_pan_mDAG=read.graph(
  paste0(path_exp,
    "TaxonomyLevels/Kingdom/Animals/pan/Animals_pan_mDAG.graphml"),
  format = "graphml")
summary(graph_pan_mDAG)
```

```
IGRAPH 6247495 D--- 1184 1261 --
+ attr: color (v/c), label (v/c), id (v/c), id (e/c)
```

The graph pan mDAG have 1184 vertex and 1261.

2.3.2 Pan Reaction graph (RC)

```
graph_pan_RC=read.graph(
  paste0(path_exp,
    "TaxonomyLevels/Kingdom/Animals/pan/Animals_pan_RC.graphml"),
  format = "graphml")
summary(graph_pan_RC)
```

```
IGRAPH 624d9bb D--- 4556 5798 --
+ attr: color (v/c), label (v/c), id (v/c), id (e/c)
```

The graph pan reaction graph have 4556 vertex and 5798.

```
compo=components(graph_mDAG, mode = "weak")
str(compo)

List of 3
$ membership: num [1:1026] 1 1 1 1 1 1 1 1 1 ...
$ csize      : num [1:167] 589 1 1 1 1 1 4 3 4 3 ...
$ no         : int 167

compo$csize
```

```

[1] 589   1   1   1   1   1   1   4   3   4   3   2   3   3   1   1   1   1   2   6
[19]   3   1   3   6   1   1   1   1   1   3   1   6   2   1   1   1   1   1   1   2   1
[37]   1  14   1  16   1   6   2   2   4   1   1   1   1   1   1   1   1   1   1   1
[55]  13   1   1   1   1   2   6   5   5   2   2   10  1   1   1   1   1   2   2   1
[73]   1   1  62   6   2   1   2   1   1   1   2   1   2   1   2   14  3   1   1   1
[91]   1   1   1   1   1   1   3   6   1   3   1   3   2   1   1   2   3   4   1   1   2
[109]   3   1   1   2   5   1   1   2   3   2   1   1   2   3   4   1   1   1   2   2
[127]   1   1   2   1   1   1   3   1   2   2   1   6   1   1   1   2   1   3   1
[145]   1   1   1   1   1   2   7   1  15  3   1   1   1   1   2   1   3   1
[163]   1   1   1   1   2

```

```

k=which.max(compo$csizes==max(compo$csizes))
k

```

```
[1] 1
```

```
table(compo$membership)
```

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
589	1	1	1	1	1	4	3	4	3	2	3	3	1	1	1	1	2	6	3	1
21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	
3	6	1	1	1	1	1	3	1	6	2	1	1	1	2	1	1	14	1	16	
41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	
1	6	2	2	4	1	1	1	1	1	1	1	1	1	13	1	1	1	1	2	
61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	
6	5	5	2	2	10	1	1	1	2	2	1	1	1	62	6	2	1	2	1	
81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	
1	1	2	1	2	14	3	1	1	1	1	1	1	1	1	1	1	3	6	1	3
101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	
1	3	2	1	1	1	2	2	3	1	1	2	5	1	1	2	3	2	1	1	
121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	
2	3	4	1	1	2	1	1	2	1	1	1	1	1	3	1	2	2	1	6	
141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	
1	1	1	2	1	1	1	1	1	2	7	1	15	3	1	1	1	1	2	1	
161	162	163	164	165	166	167														
3	1	1	1	1	1	1	2													

```

vertex=which(compo$membership==k)
length(vertex)

```

```
[1] 589
```

```
Big_Component=induced_subgraph(graph_mDAG, vids=vertex)
igraph::vcount(Big_Component)
```

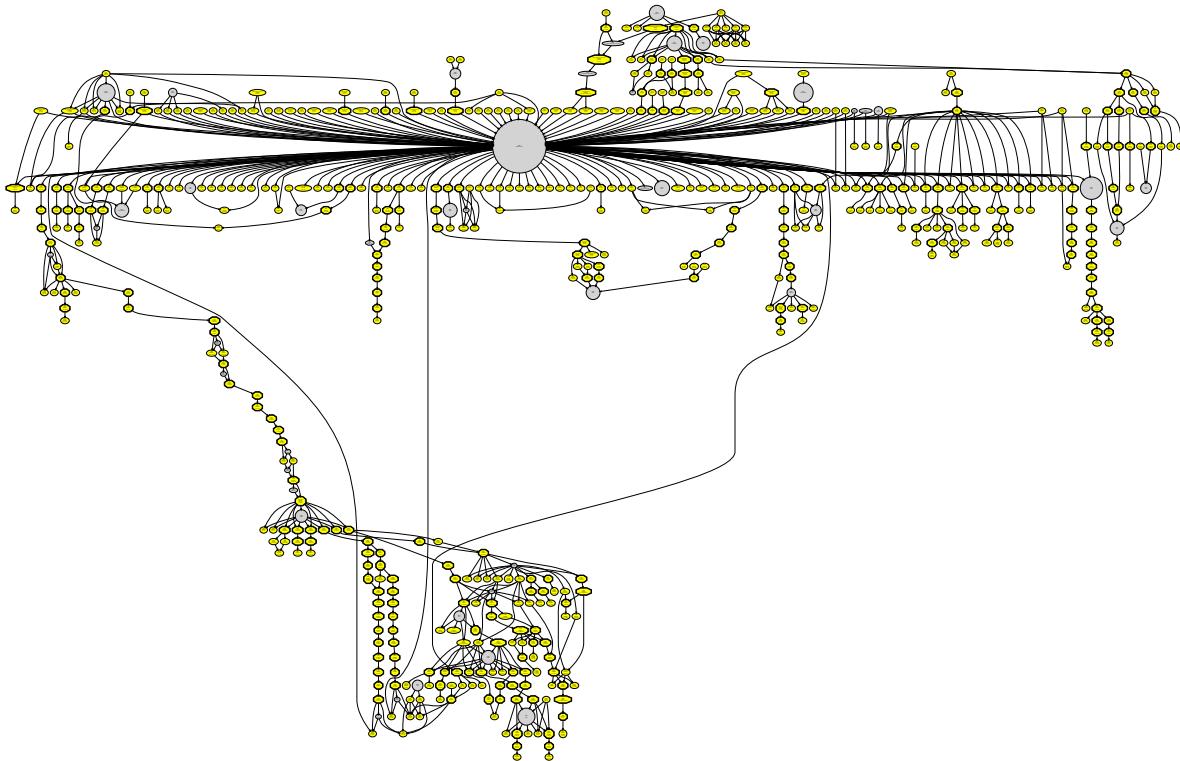
```
[1] 589
```

```
igraph::ecount(Big_Component)
```

```
[1] 774
```

The curated plot of the bigger component of hsa mDAG

```
knitr:::include_graphics(paste0(path_exp,
"Individuals/hsa/hsa_mDAG_biggerDAG.pdf"))
```



3 Similarities and metadata for an experiment

We will first load the metadata and adapt them to the structure of the similarities to facilitate the creation of the graphs and statistics.

Remember de path of the experiment:

```
path_exp
```

```
[1] "data/result_0c982fc3-a45f-3645-b0b9-989a0425da6a/data/"
```

3.1 Load meta data from eukariotes experimet

Meta data mDa_Id and taxonomy sort by Kingdom,Filum,Class,mDAG_Id

```
path_exp
```

```
[1] "data/result_0c982fc3-a45f-3645-b0b9-989a0425da6a/data/"
```

```
Results=read_csv(paste0(path_exp,"Results.csv"))
#arreglo los nombres de MEtaDag
names(Results)[c(1,2,3,4,5)]=c("Organism","Categories","Groups","mDAG_Id","Full_Name")
taxo=Results %>% select(Organism:Full_Name)
taxo=taxo %>% separate(Categories,into=c("Kingdom","Phylum","Class"))
index=which(is.na(taxo$Class))
taxo$Class[index]=paste(taxo$Phylum[index])
meta_taxo=taxo
aux=table(meta_taxo$Phylum)
Freq_Phylum=tibble(Phylum=names(aux),Freq_Phylum=aux)
names(Freq_Phylum)=c("Phylum","Freq_Phylum")
aux=table(meta_taxo$Class)
Freq_Class=tibble(Class=names(aux),Freq_Class=aux)
names(Freq_Class)=c("Class","Freq_Class")

meta_taxo = meta_taxo %>%
```

```

  left_join(Freq_Phylum) %>%
  left_join(Freq_Class)
meta_taxo = meta_taxo %>%
  arrange(Kingdom,desc(Freq_Phylum),Phylum,
          desc(Freq_Class),Class)
head(meta_taxo)

# A tibble: 6 x 9
  Organism Kingdom Phylum Class Groups mDAG_Id Full_Name Freq_Phylum Freq_Class
  <chr>     <chr>   <chr>  <chr> <chr>    <chr>      <table[1d]> <table[1d>
1 aamp      Animals Vertebr Mamm Clust~ 0313     Arvicola~ 331      139
2 afz       Animals Vertebr Mamm Clust~ 0143     Antechin~ 331      139
3 ajm       Animals Vertebr Mamm Clust~ 0221     Artibeus~ 331      139
4 aju       Animals Vertebr Mamm Clust~ 0224     Acinonyx~ 331      139
5 aml       Animals Vertebr Mamm Clust~ 0279     Ailuropo~ 331      139
6 anu       Animals Vertebr Mamm Clust~ 0310     Arvican~ 331      139

table(meta_taxo$Kingdom) %>% kable %>%
  kable_styling("striped", full_width = F,position="left")%>%
  scroll_box(width = "400px", height = "200px")



| Var1     | Freq |
|----------|------|
| Animals  | 535  |
| Fungi    | 154  |
| Plants   | 139  |
| Protists | 56   |



table(meta_taxo$Phylum,meta_taxo$Kingdom) %>% kable %>%
  kable_styling("striped", full_width = F,position="left")%>%
  scroll_box(width = "500px", height = "500px")

```

	Animals	Fungi	Plants	Protists
Alveolates	0	0	0	25
Amoebozoa	0	0	0	7
Annelids	1	0	0	0
Arthropods	158	0	0	0
Ascomycetes	0	113	0	0
Basal	0	0	2	0
Basidiomycetes	0	36	0	0
Brachiopoda	1	0	0	0
Cephalochordates	2	0	0	0
Choanoflagellates	0	0	0	2
Cnidarians	10	0	0	0
Cryptomonads	0	0	0	1
Echinoderms	3	0	0	0
Eudicots	0	0	98	0
Euglenozoa	0	0	0	9
Ferns	0	0	1	0
Flatworms	4	0	0	0
Green	0	0	11	0
Haptophyta	0	0	0	1
Hemichordates	1	0	0	0
Heterolobosea	0	0	0	1
Metamonada	0	0	0	2
Microsporidians	0	5	0	0
Mollusks	14	0	0	0
Monocots	0	0	23	0
Mosses	0	0	1	0
Nematodes	6	0	0	0
Placozoans	1	0	0	0
Poriferans	1	0	0	0
Red	0	0	3	0
Stramenopiles	0	0	0	8
Tunicates	2	0	0	0
Vertebrates	331	0	0	0

3.2 Similarities MSA,Munkres methods

In this section we will show the similarities between mDAG's using different methods.

The experiment data set consists of 884 eukaryotes from the animal, plant, fungus, and protist kingdoms.

Kingdom	Abs. Freq.
Animals	535
Fungi	154
Plants	139
Protists	56

```
list_Sim=dir(path_exp,pattern="^Similarities")
list_Sim

[1] "Similarities_MBB_MSAMethod.csv"      "Similarities_MBB_MunkresMethod.csv"
[3] "Similarities_mDAG_MSAMethod.csv"     "Similarities_mDAG_MunkresMethod.csv"
```

Load MDAG similarities

```
Sim_MSA_mDAG=read_csv(paste0(path_exp,
                               "Similarities_mDAG_MSAMethod.csv"))
Sim_MSA_mDAG=as.matrix(Sim_MSA_mDAG[,-1])
rownames(Sim_MSA_mDAG)=colnames(Sim_MSA_mDAG)
Sim_MSA_mDAG=Sim_MSA_mDAG[meta_taxo$mDAG_Id,meta_taxo$mDAG_Id]

Sim_Mun_mDAG=read_csv(paste0(path_exp,"Similarities_mDAG_MunkresMethod.csv"))
Sim_Mun_mDAG=as.matrix(Sim_Mun_mDAG[,-1])
rownames(Sim_Mun_mDAG)=colnames(Sim_Mun_mDAG)
Sim_Mun_mDAG=Sim_Mun_mDAG[meta_taxo$mDAG_Id,meta_taxo$mDAG_Id]
```

3.3 Heatmaps

3.3.1 Heatmap Similarity MSA and Munkres method

```
dff<-meta_taxo %>% select(Kingdom)  %>% as.data.frame()
colorsK <- list(Kingdom= c("Animals"="red",
                           "Plants"="green",
                           "Fungi"="yellow",
                           "Protists"="black"))
annotationK <- HeatmapAnnotation(df=dff, col = colorsK,show_legend = TRUE)

MSA_heat_1 <- Heatmap(matrix = Sim_MSA_mDAG,
                      column_title=
                        "m-DAGs MSA-similarity Eukaryotes by Kingdoms",
                      heatmap_legend_param=list(
                        title="Similarity",
```

```

        at = seq(0,1,by=0.1)),
        col=rev(viridis(256)),
        cluster_rows = FALSE,
        cluster_columns = FALSE,
        top_annotation = annotationK,
        show_column_names = FALSE,
        show_row_names = FALSE,
        left_annotation =
          rowAnnotation(df = df,
                        col = colorsK,
                        show_annotation_name=FALSE,
                        show_legend=FALSE
                      )))

```

```

Mun_heat_1<- Heatmap(matrix = Sim_Mun_mDAG,
                      column_title="mDAGs Munkres-similarity Eukaryotes by Kingdoms",
                      name = "Munkres Similarity",
                      heatmap_legend_param=list(
                        title="Similarity",
                        at = seq(0,1,by=0.1)),
                        col=rev(viridis(256)),
                        cluster_rows = FALSE,
                        cluster_columns = FALSE,
                        top_annotation = annotationK,
                        show_column_names = FALSE,
                        show_row_names = FALSE,
                        left_annotation =
                          rowAnnotation(df = df,
                            col = colorsK,
                            show_annotation_name=FALSE,
                            show_legend=FALSE
                          )))

```

```

meta_animals= meta_taxo %>% filter(Kingdom=="Animals")

dff<-meta_taxo %>%
  filter(Kingdom=="Animals") %>%

```

```

select(Phylum,Freq_Phylum) %>%
as.data.frame() %>% select(Phylum)

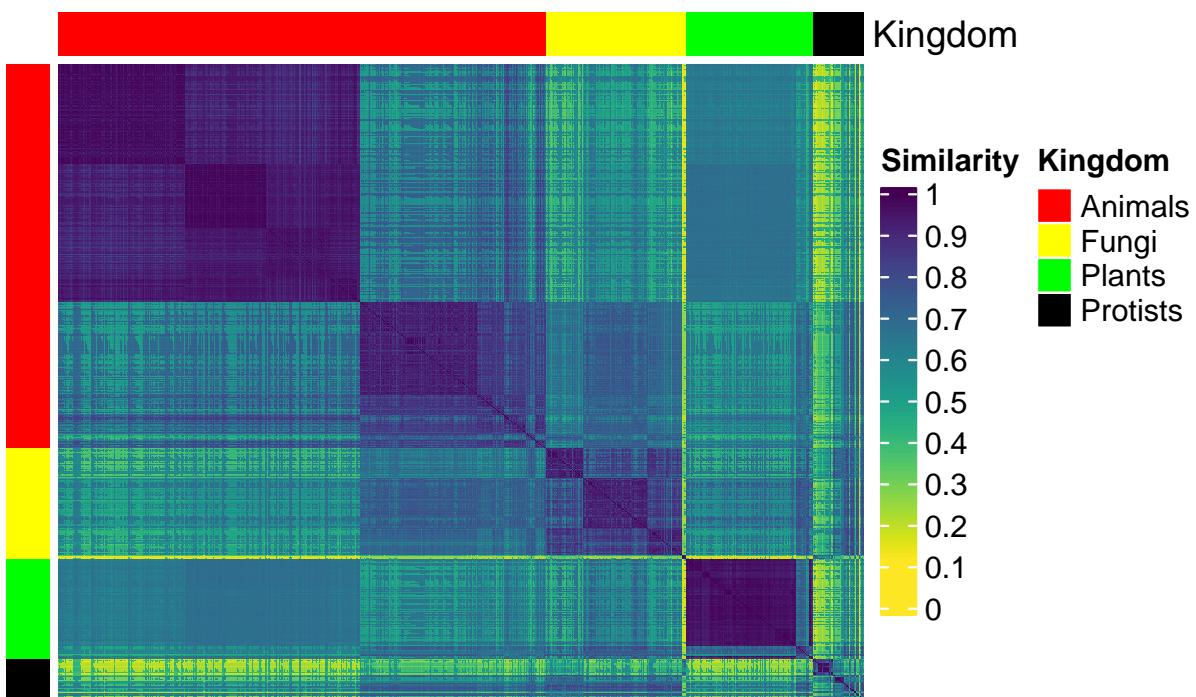
namesP=dff %>% distinct( Phylum, .keep_all = TRUE)
namesP=namesP$Phylum
dff$Phylum=ordered(dff$Phylum,labels=namesP)
col=rainbow(length(namesP))
colorsP=list(Phylum=col)
names(colorsP$Phylum)=namesP
annotation_H2 <- HeatmapAnnotation(df=dff, col = colorsP)
MSA_heat_2 <- Heatmap(matrix =
  Sim_MSA_mDAG[1:nrow(dff),1:nrow(dff)],
  column_title="mDAGs MSA-similarity Animals by Phyla",
  col=rev(viridis(256)),
  cluster_rows = FALSE,
  show_heatmap_legend=FALSE,
  cluster_columns = FALSE,
  top_annotation = annotation_H2,
  show_column_names = FALSE,
  show_row_names = FALSE,
  left_annotation =
    rowAnnotation(df = dff,
                  col = colorsP,
                  show_annotation_name=FALSE,
                  show_legend =FALSE
                ))
))

Mun_heat_2 <- Heatmap(matrix = Sim_Mun_mDAG[1:nrow(dff),1:nrow(dff)],
  column_title="mDAGs Munkres-similarity Animals by Phyla",
  col=rev(viridis(256)),
  show_heatmap_legend=FALSE,
  cluster_rows = FALSE,
  cluster_columns = FALSE,
  top_annotation = annotation_H2,
  show_column_names = FALSE,
  show_row_names = FALSE,
  left_annotation = rowAnnotation(df = dff,
                                    col = colorsP,
                                    show_annotation_name=FALSE,
                                    show_legend =FALSE
                                  ))
)

```

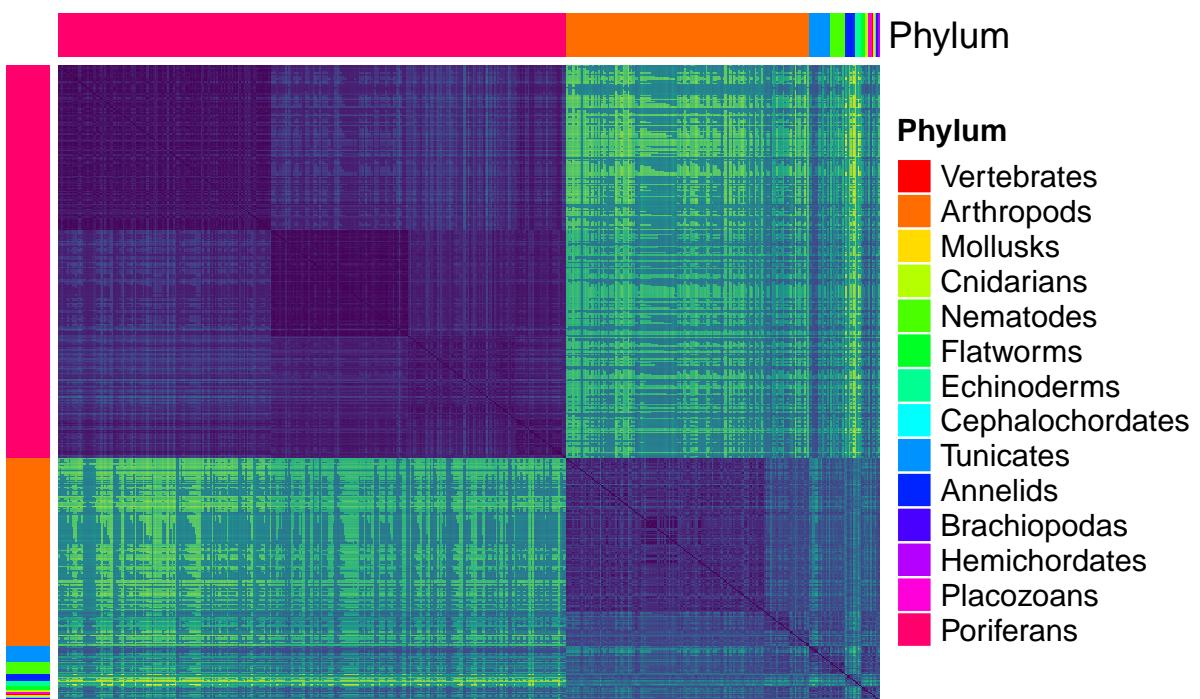
MSA_heat_1

m-DAGs MSA-similarity Eukaryotes by Kingdoms



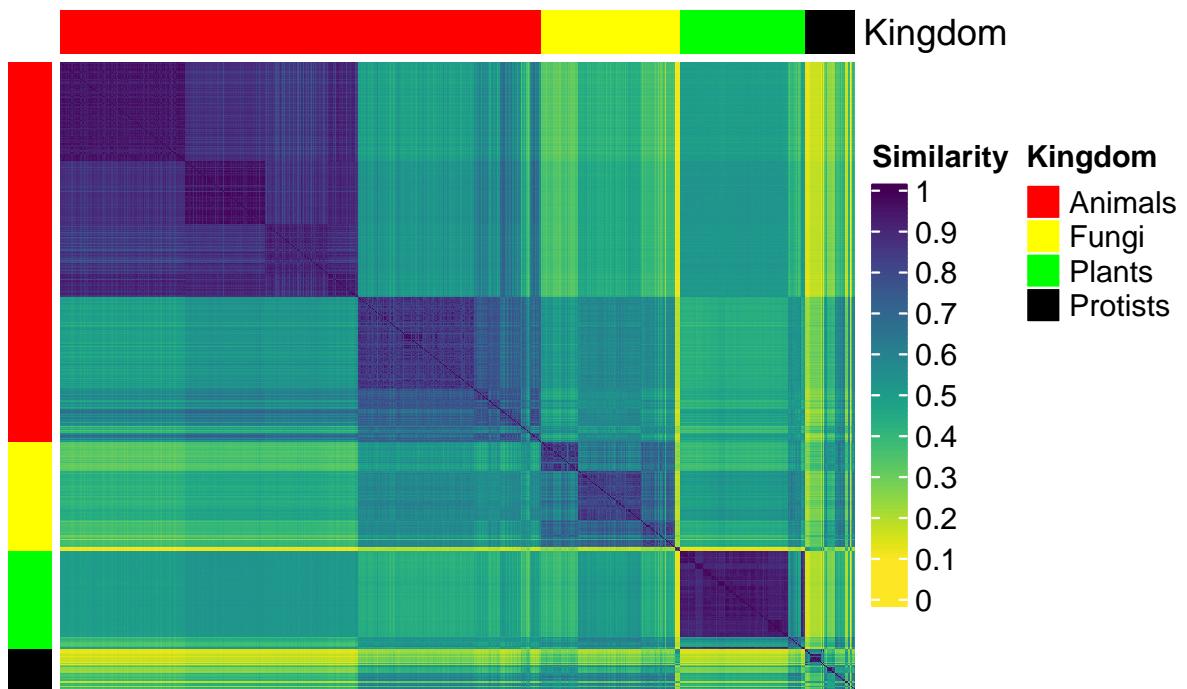
MSA_heat_2

mDAGs MSA–similarity Animals by Phyla



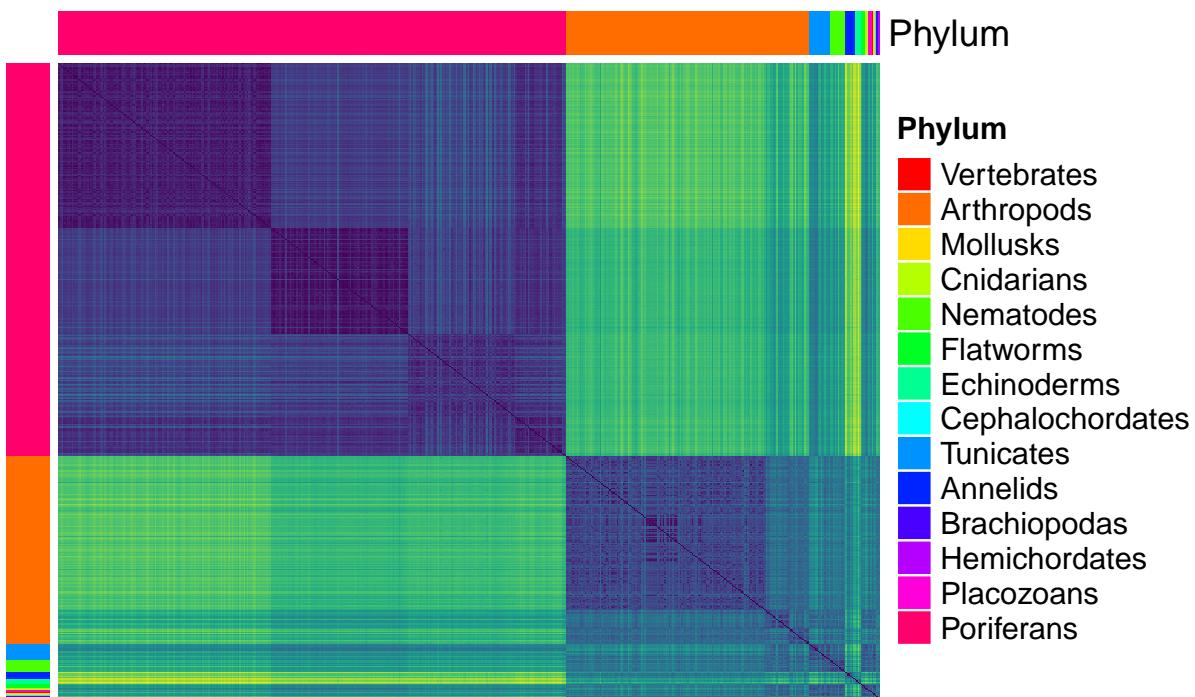
Mun_heat_1

mDAGs Munkres–similarity Eukaryotes by Kingdoms



Mun_heat_2

mDAGs Munkres–similarity Animals by Phyla



3.4 MDS (Multidimensional Scaling) MSA

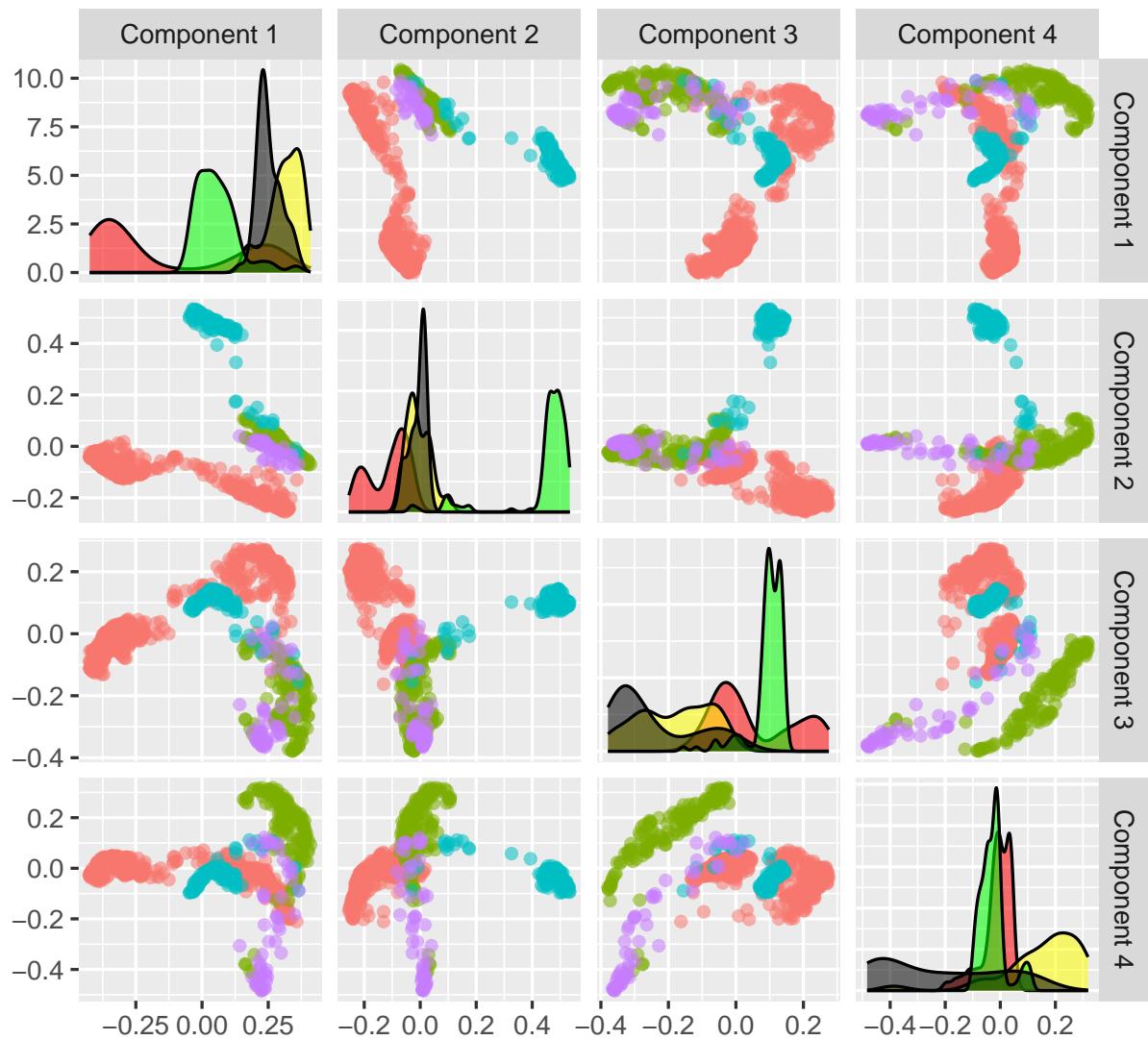
```
## Metric multidimensional scaling (mMDS)
mds7 <- cmdscale(sqrt(1-Sim_MSA_mDAG^2), k=7, eig=TRUE)
#pairs(mds7$points[,1:4])
mds7$GOF

[1] 0.4449519 0.5570199

mds <- mds7$points %>% as_tibble()
colnames(mds) <- paste0("Dim.", 1:dim(mds7$points)[2])

cooordinates=as_tibble(mds7$points)
colnames(cooordinates)=paste("Component", 1:7)
ggpairs(cooordinates, columns=1:4,
        aes(color=meta_taxo$Kingdom, alpha=0.5,
            title="MDS 4 dimensions projection",
            legend=1), upper=list(continuous="points")) +
```

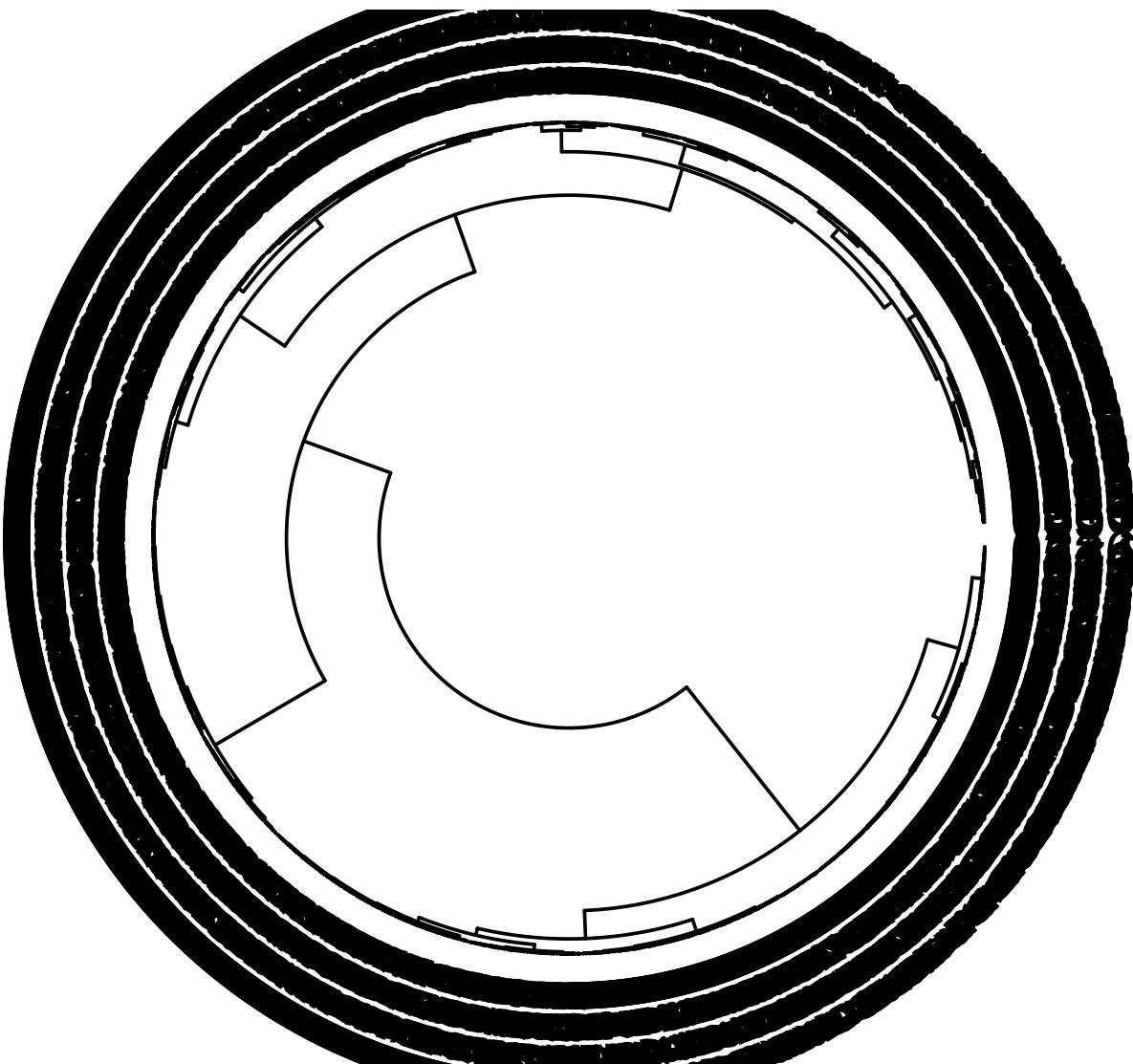
```
scale_fill_manual(values = colorsK$Kingdom) +  
theme(legend.position = "left")
```



4 Hierarchical cluster MSA

```
library(dendextend)
library(ggraph)
library(ape)

D=as.dist(sqrt(1-Sim_MSA_mDAG^2))
hc_MSA=hclust(as.dist(D),method ="ward.D")
library(circlize)
circlize_dendrogram(as.dendrogram(hc_MSA))
```



```
clust4_MSA=cutree(hc_MSA,4)
table(clust4_MSA,meta_taxo$Kingdom)
```

clust4_MSA	Animals	Fungi	Plants	Protists
1	331	0	0	0
2	197	0	0	0
3	7	154	14	56
4	0	0	125	0

```
aux=meta_taxo %>%
  select(Organism,Kingdom,Phylum,Class,Full_Name)
```

```

aux$clust4_MSA=clust4_MSA
aux_Animals_cluster_1_2 = aux %>%
  filter(Kingdom=="Animals",clust4_MSA %in% c(1,2))

```

```
table(aux_Animals_cluster_1_2$Phylum,aux_Animals_cluster_1_2$clust4_MSA)
```

	1	2
Annelids	0	1
Arthropods	0	158
Brachiopodas	0	1
Cephalochordates	0	2
Cnidarians	0	10
Echinoderms	0	3
Hemichordates	0	1
Mollusks	0	14
Nematodes	0	3
Placozoans	0	1
Poriferans	0	1
Tunicates	0	2
Vertebrates	331	0

```

aux_9_Animals_cluster_3= filter(aux,
                                 clust4_MSA==3,
                                 Kingdom=="Animals")
aux_9_Animals_cluster_3

```

```

# A tibble: 7 x 6
  Organism Kingdom Phylum   Class      Full_Name       clust4_MSA
  <chr>     <chr>   <chr>    <chr>    <chr>           <int>
1 bmy       Animals Nematodes Nematodes Brugia malayi (filaria)      3
2 loa       Animals Nematodes Nematodes Loa loa (eye worm)            3
3 tsp       Animals Nematodes Nematodes Trichinella spiralis          3
4 egl       Animals Flatworms Flatworms Echinococcus granulosus (hyda~ 3
5 ovi       Animals Flatworms Flatworms Opisthorchis viverrini (South~ 3
6 shx       Animals Flatworms Flatworms Schistosoma haematobium (urin~ 3
7 smm       Animals Flatworms Flatworms Schistosoma mansoni             3

```

```

aux_all_Nematodes_Flatworns= aux %>%
  filter(Kingdom=="Animals",
         Phylum %in% c("Nematodes", "Flatworms"))
aux_all_Nematodes_Flatworns

```

```

# A tibble: 10 x 6
  Organism Kingdom Phylum   Class Full_Name      clust4_MSA
  <chr>     <chr>   <chr>   <chr>   <chr>           <int>
1 bmy       Animals Nematodes Nematodes Brugia malayi (filaria) 3
2 cbr       Animals Nematodes Nematodes Caenorhabditis briggsae (nem~ 2
3 cel       Animals Nematodes Nematodes Caenorhabditis elegans (nema~ 2
4 loa       Animals Nematodes Nematodes Loa loa (eye worm)        3
5 nai       Animals Nematodes Nematodes Necator americanus (New Worl~ 2
6 tsp       Animals Nematodes Nematodes Trichinella spiralis        3
7 egl       Animals Flatworms Flatworms Echinococcus granulosus (hyd~ 3
8 ovi       Animals Flatworms Flatworms Opisthorchis viverrini (Sout~ 3
9 shx       Animals Flatworms Flatworms Schistosoma haematobium (uri~ 3
10 smm      Animals Flatworms Flatworms Schistosoma mansoni         3

aux_14_Plants_clust2= filter(aux,clust4_MSA==3,
                               Kingdom=="Plants")
aux_14_Plants_clust2

# A tibble: 14 x 6
  Organism Kingdom Phylum Class Full_Name      clust4_MSA
  <chr>     <chr>   <chr>   <chr>   <chr>           <int>
1 apro      Plants  Green   algae Auxenochlorella protothecoides 3
2 bpg       Plants  Green   algae Bathycoccus prasinos        3
3 cre       Plants  Green   algae Chlamydomonas reinhardtii 3
4 csl       Plants  Green   algae Coccomyxa subellipsoidea 3
5 cvr       Plants  Green   algae Chlorella variabilis        3
6 mis       Plants  Green   algae Micromonas commoda        3
7 mng       Plants  Green   algae Monoraphidium neglectum 3
8 mpp       Plants  Green   algae Micromonas pusilla        3
9 olu       Plants  Green   algae Ostreococcus lucimarinus 3
10 ota      Plants  Green   algae Ostreococcus tauri        3
11 vcn      Plants  Green   algae Volvox carteri f. nagariensis 3
12 ccp      Plants  Red    algae Chondrus crispus (carragheen) 3
13 cme      Plants  Red    algae Cyanidioschyzon merolae        3
14 gsl      Plants  Red    algae Galdieria sulphuraria        3

aux_all_algae_class= aux %>%
  filter(Kingdom=="Plants",
         Class %in% c("algae"))
aux_all_algae_class

# A tibble: 14 x 6

```

	Organism	Kingdom	Phylum	Class	Full_Name	clust4_MSA
	<chr>	<chr>	<chr>	<chr>	<chr>	<int>
1	apro	Plants	Green	algae	Auxenochlorella protothecoides	3
2	bpg	Plants	Green	algae	Bathycoccus prasinos	3
3	cre	Plants	Green	algae	Chlamydomonas reinhardtii	3
4	csl	Plants	Green	algae	Coccomyxa subellipsoidea	3
5	cvr	Plants	Green	algae	Chlorella variabilis	3
6	mis	Plants	Green	algae	Micromonas commoda	3
7	mng	Plants	Green	algae	Monoraphidium neglectum	3
8	mpp	Plants	Green	algae	Micromonas pusilla	3
9	olu	Plants	Green	algae	Ostreococcus lucimarinus	3
10	ota	Plants	Green	algae	Ostreococcus tauri	3
11	vcn	Plants	Green	algae	Volvox carteri f. nagariensis	3
12	ccp	Plants	Red	algae	Chondrus crispus (carragheen)	3
13	cme	Plants	Red	algae	Cyanidioschyzon merolae	3
14	gsl	Plants	Red	algae	Galdieria sulphuraria	3

The hierarchical classification by Ward's method recovers the kingdom Animal clusters 1 (all vertebrates) and 2 (invertebrate animals), cluster 4 the Plants and in cluster 3 are all protists and fungi together with 9 animals and 14 plants.

The 9 Animals are all from the Phylum Nematodes or Flatworms, out of the total of the 10 species of these phyla considered in the experiment. Only the Nematode Necator americanus (New World hookworm) is classified in Animals.

The 14 plants in cluster 2 are all algae considered in the experiment.

4.1 MDS (Multidimensional Scaling) Munkres

```
## Metric multidimensional scaling
mds7 <- cmdscale(sqrt(1-Sim_Mun_mDAG^2), k=7, eig=TRUE)
mds7$GOF

[1] 0.5604760 0.5800268

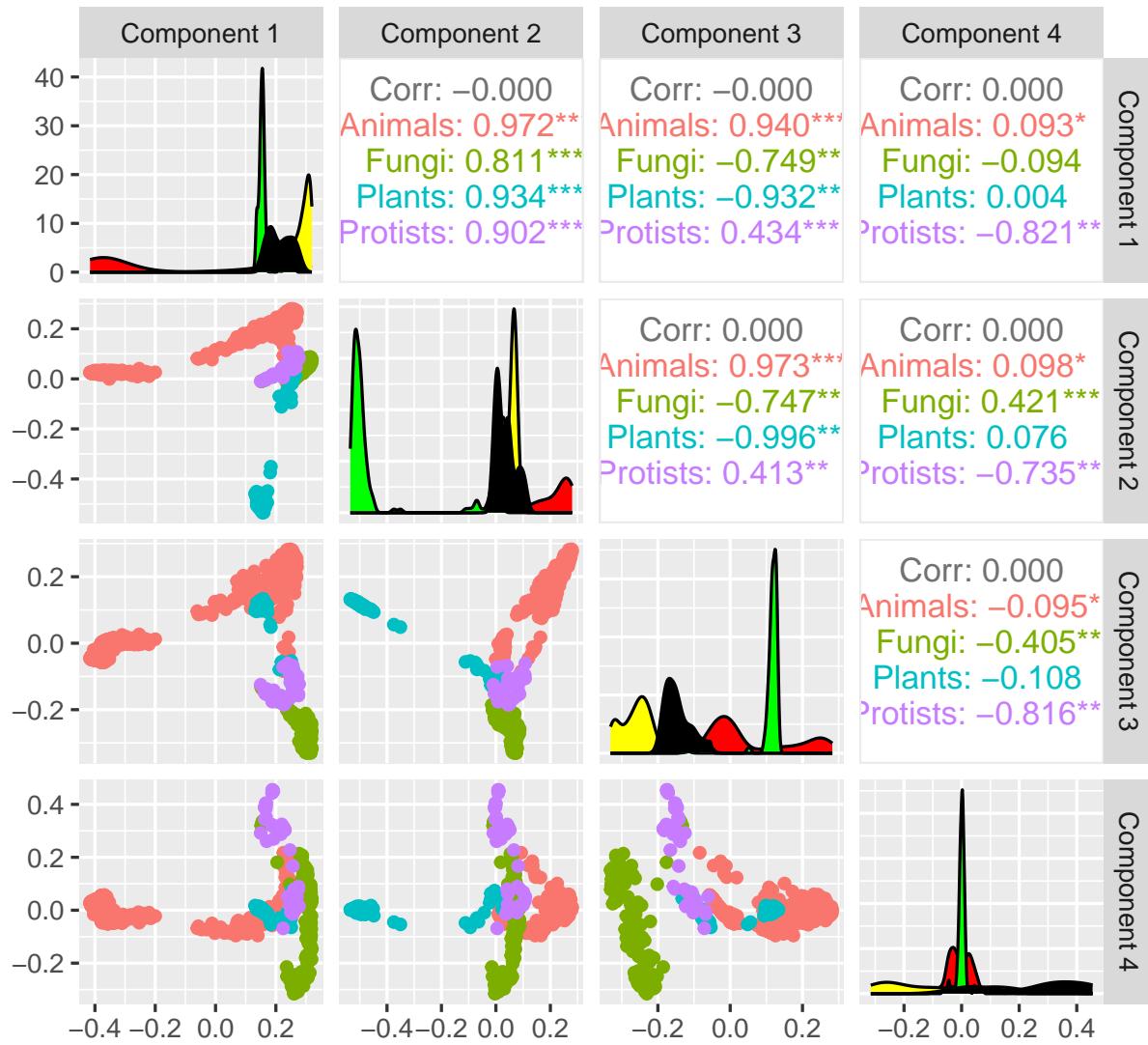
mds <- mds7$points %>% as_tibble()
colnames(mds) <- paste0("Dim.", 1:dim(mds7$points)[2])

cooordinates=as_tibble(mds7$points)
colnames(cooordinates)=paste("Component", 1:7)
ggpairs(cooordinates, columns=1:4,
        aes(color=meta_taxo$Kingdom,
```

```

    title="MDS 4 dimensions projection",legend=1),
    lower=list(continuous="points")) +
  scale_fill_manual(values = colorsK$Kingdom) +
  theme(legend.position = "left")

```

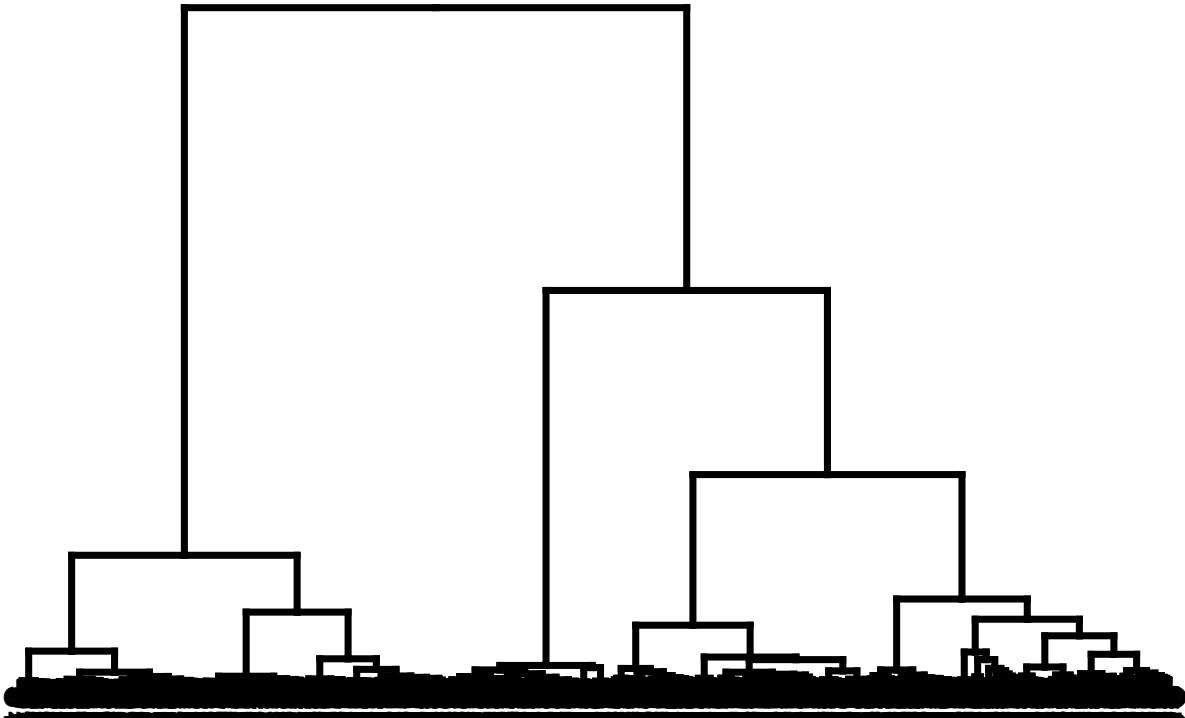


4.2 Hierarchical cluster Munkres

```

D=as.dist(sqrt(1-Sim_Mun_mDAG^2))
hc_Mun=hclust(as.dist(D),method ="ward.D")
ggplot(as.ggdend(as.dendrogram(hc_Mun)))

```



```
clust4_Mun=cutree(hc_Mun,4)
table(clust4_Mun,meta_taxo$Kingdom)
```

clust4_Mun	Animals	Fungi	Plants	Protists
1	331	0	0	0
2	197	0	0	0
3	7	154	14	56
4	0	0	125	0

Only two nematodes of the 9 return to the invertebrate animal cluster for Munkrest; all algae remain in the fungi and archaea cluster.

```
aux=meta_taxo %>%
  select(Organism,Kingdom,Phylum,Class,Full_Name)
aux$clust4_Mun=clust4_Mun
aux_Animals_cluster_1_2_Mun = aux %>%
  filter(Kingdom=="Animals",clust4_Mun %in% c(1,2))

table(aux_Animals_cluster_1_2_Mun$Phylum,
      aux_Animals_cluster_1_2_Mun$clust4_Mun)
```

	1	2
Annelids	0	1
Arthropods	0	158
Brachiopodas	0	1
Cephalochordates	0	2
Cnidarians	0	10
Echinoderms	0	3
Hemichordates	0	1
Mollusks	0	14
Nematodes	0	3
Placozoans	0	1
Poriferans	0	1
Tunicates	0	2
Vertebrates	331	0

```
aux_7_Animals_cluster_3_Mun= filter(aux,
                                      clust4_Mun==3,
                                      Kingdom=="Animals")
aux_7_Animals_cluster_3_Mun
```

```
# A tibble: 7 x 6
  Organism Kingdom Phylum   Class Full_Name      clust4_Mun
  <chr>     <chr>   <chr>    <chr>   <chr>          <int>
1 bmy       Animals Nematodes Nematodes Brugia malayi (filaria) 3
2 loa       Animals Nematodes Nematodes Loa loa (eye worm)      3
3 tsp       Animals Nematodes Nematodes Trichinella spiralis    3
4 egl       Animals Flatworms Flatworms Echinococcus granulosus (hyda~ 3
5 ovi       Animals Flatworms Flatworms Opisthorchis viverrini (South~ 3
6 shx       Animals Flatworms Flatworms Schistosoma haematobium (urin~ 3
7 smm       Animals Flatworms Flatworms Schistosoma mansoni        3
```

```
aux_all_Nematodes_Flatworns= aux %>%
  filter(Kingdom=="Animals",
         Phylum %in% c("Nematodes", "Flatworms"))
aux_all_Nematodes_Flatworns
```

```
# A tibble: 10 x 6
  Organism Kingdom Phylum   Class Full_Name      clust4_Mun
  <chr>     <chr>   <chr>    <chr>   <chr>          <int>
1 bmy       Animals Nematodes Nematodes Brugia malayi (filaria) 3
2 cbr       Animals Nematodes Nematodes Caenorhabditis briggsae (nem~ 2
```

```

3 cel      Animals Nematodes Nematodes Caenorhabditis elegans (nema~ 2
4 loa      Animals Nematodes Nematodes Loa loa (eye worm)            3
5 nai      Animals Nematodes Nematodes Necator americanus (New Worl~ 2
6 tsp      Animals Nematodes Nematodes Trichinella spiralis           3
7 egl      Animals Flatworms Flatworms Echinococcus granulosus (hyd~ 3
8 ovi      Animals Flatworms Flatworms Opisthorchis viverrini (Sout~ 3
9 shx      Animals Flatworms Flatworms Schistosoma haematobium (uri~ 3
10 smm     Animals Flatworms Flatworms Schistosoma mansoni             3

aux_14_Plants_clust2_Mun= filter(aux,clust4_Mun==3,
                                   Kingdom=="Plants")
aux_14_Plants_clust2_Mun

# A tibble: 14 x 6
  Organism Kingdom Phylum Class Full_Name                  clust4_Mun
  <chr>    <chr>   <chr>  <chr> <chr>                    <int>
1 apro     Plants  Green  algae Auxenochlorella protothecoides       3
2 bpg      Plants  Green  algae Bathycoccus prasinos                 3
3 cre      Plants  Green  algae Chlamydomonas reinhardtii            3
4 csl      Plants  Green  algae Coccomyxa subellipsoidea            3
5 cvr      Plants  Green  algae Chlorella variabilis                3
6 mis      Plants  Green  algae Micromonas commoda                 3
7 mng      Plants  Green  algae Monoraphidium neglectum              3
8 mpp      Plants  Green  algae Micromonas pusilla                 3
9 olu      Plants  Green  algae Ostreococcus lucimarinus            3
10 ota     Plants  Green  algae Ostreococcus tauri                  3
11 vcn     Plants  Green  algae Volvox carteri f. nagariensis        3
12 ccp      Plants  Red    algae Chondrus crispus (carragheen)          3
13 cme     Plants  Red    algae Cyanidioschyzon merolae               3
14 gsl      Plants  Red    algae Galdieria sulphuraria              3

aux_all_algae_class= aux %>%
  filter(Kingdom=="Plants",
         Class %in% c("algae"))
aux_all_algae_class

# A tibble: 14 x 6
  Organism Kingdom Phylum Class Full_Name                  clust4_Mun
  <chr>    <chr>   <chr>  <chr> <chr>                    <int>
1 apro     Plants  Green  algae Auxenochlorella protothecoides       3
2 bpg      Plants  Green  algae Bathycoccus prasinos                 3
3 cre      Plants  Green  algae Chlamydomonas reinhardtii            3

```

4	csl	Plants	Green	algae	Coccomyxa subellipsoidea	3
5	cvr	Plants	Green	algae	Chlorella variabilis	3
6	mis	Plants	Green	algae	Micromonas commoda	3
7	mng	Plants	Green	algae	Monoraphidium neglectum	3
8	mpp	Plants	Green	algae	Micromonas pusilla	3
9	olu	Plants	Green	algae	Ostreococcus lucimarinus	3
10	ota	Plants	Green	algae	Ostreococcus tauri	3
11	vcn	Plants	Green	algae	Volvox carteri f. nagariensis	3
12	ccp	Plants	Red	algae	Chondrus crispus (carragheen)	3
13	cme	Plants	Red	algae	Cyanidioschyzon merolae	3
14	gsl	Plants	Red	algae	Galdieria sulphuraria	3

4.3 Similarity comparison Eukaryotes

Comparison of two similarities

Load the similarities for pairs and comparison

```
n=length(meta_taxo$mDAG_Id)
n

[1] 884

dim(Sim_MSA_mDAG)

[1] 884 884

#aux1=base::rep(x=1:n, each=c(n:1))

aux=as_tibble(Sim_MSA_mDAG)
aux$mDag=names(aux)
aux=aux %>% pivot_longer(cols=`0313`:`0300`,
                           names_to="mDag_2",
                           values_to="Sim_MSA")

aux_2= aux %>% mutate(i=pmax(as.integer(mDag),
                               as.integer(mDag_2)),
                           j=pmin(as.integer(mDag),
                               as.integer(mDag_2))) %>% unite("ij",i:j) %>%
filter(duplicated(ij))
```

```

aux=as_tibble(Sim_Mun_mDAG)
aux$mDag=names(aux)
aux=aux %>% pivot_longer(cols=`0313`:`0300`,
                           names_to="mDag_2",
                           values_to="Sim_Mun")
aux_2 = aux_2 %>% left_join(aux)

Sim_comp=aux_2
rm(aux,aux_2)

```

Spearman and Pearson correlations

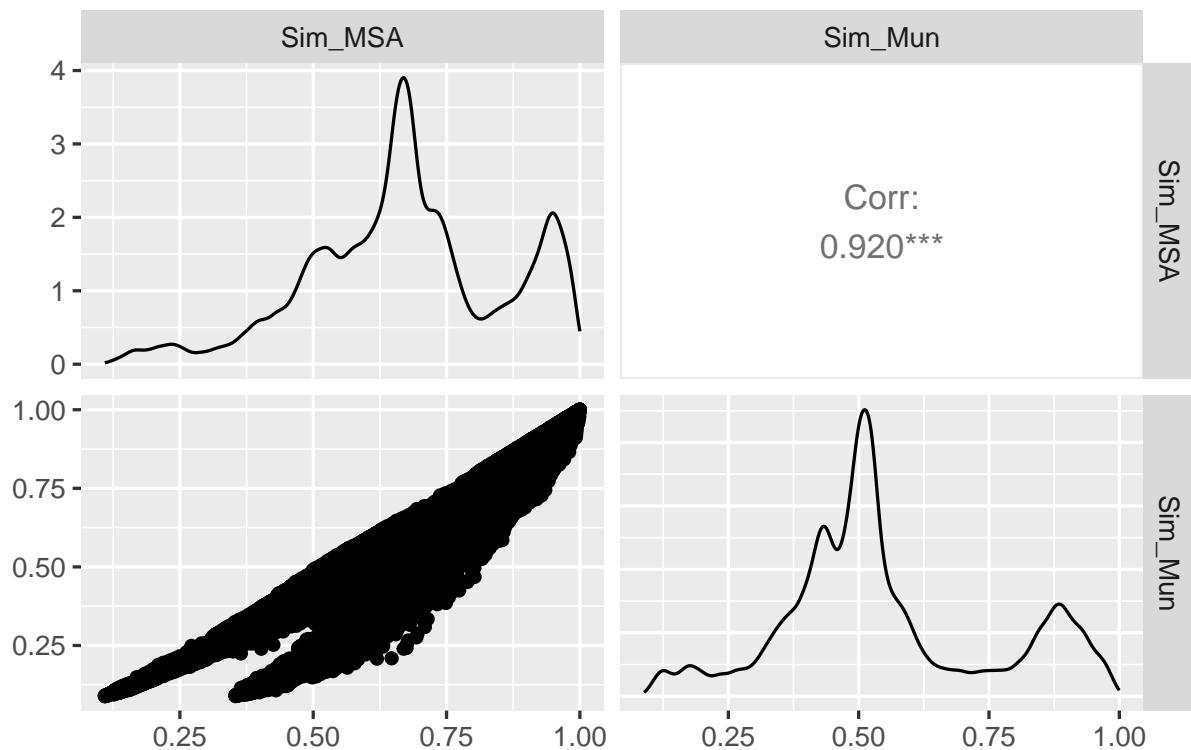
```
cor(Sim_comp[,c(3,5)],method="spearman")
```

	Sim_MSA	Sim_Mun
Sim_MSA	1.0000000	0.8930465
Sim_Mun	0.8930465	1.0000000

```
cor(Sim_comp[,c(3,5)],method="pearson")
```

	Sim_MSA	Sim_Mun
Sim_MSA	1.0000000	0.9203673
Sim_Mun	0.9203673	1.0000000

```
GGally::ggpairs(Sim_comp[,c(3,5)])
```



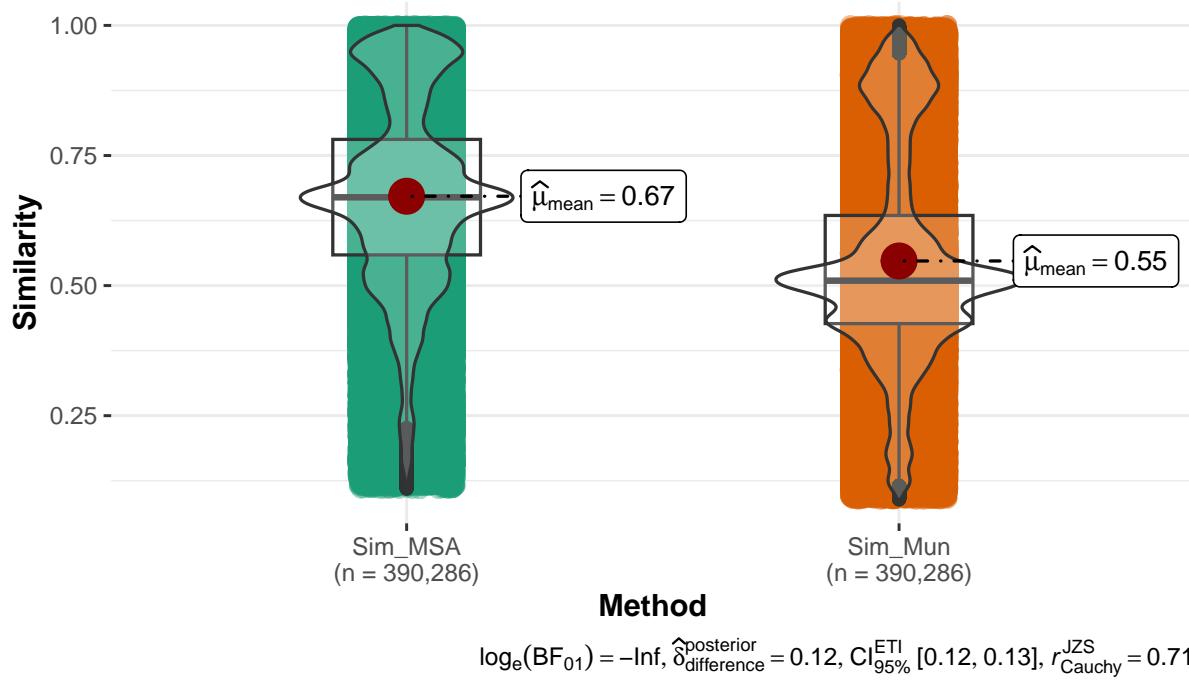
```

aux= Sim_comp%>% pivot_longer(
  cols=c(Sim_MSA,Sim_Mun),
  names_to="Method",
  values_to="Similarity")

ggstatsplot::ggbetweenstats(
  data = aux,
  x = Method,
  y = Similarity,
  centrality.plotting=TRUE)

```

$$t_{\text{Welch}}(773000) = 286.19, p = 0.00, \hat{g}_{\text{Hedges}} = 0.65, \text{CI}_{95\%} [\text{NA}, \text{NA}], n_{\text{obs}} = 780,572$$



5 Graph

Some statistics for graphs

5.1 Read all graphs from a level of the experiment

Read all graphs from a level from experiment; for example individuals. We read only first (alphabetic) two graph

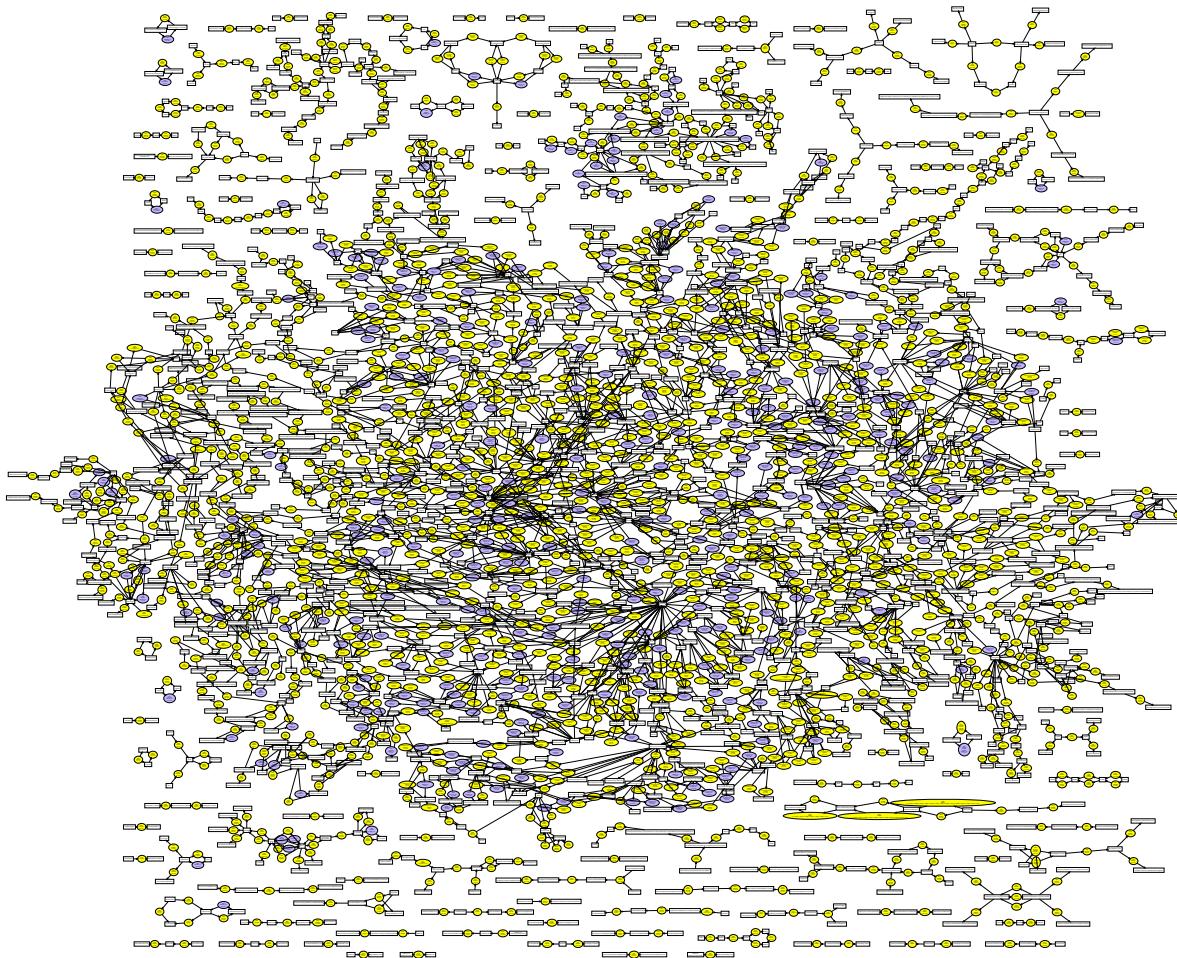
```
path_exp="data/result_bb261b6e-95c6-3e39-b82b-b68eea80e30b/data/"
list_names=dir(paste0(path_exp,"Individuals/"))

list_names= list_names[-1] # filter 0000_RefPw
length(list_names)
```

```
[1] 884
```

```
graphs_list=paste0(path_exp,"Individuals/",
                     list_names,"/",list_names,
                     "_MDAG.graphml")

knitr:::include_graphics(
  paste0(path_exp,"Individuals/cang/cang_RC.pdf"))
```



5.2 Graph statistics

```

read_mDAG=function(x) {DAG=read.graph(file=x,
                                         format="graphml")
  return(DAG)}
mDAG_componets=function(x) {
  sort(components(x,mode = "weak")$csizes,
       decreasing=TRUE)
}

compo_list=lapply(graphs_list,
                  FUN=function(x) {
                    gg=read_mDAG(x)

```

```

    aux=list(
      mDAG_componets=mDAG_componets(gg),
      degree_count=igraph::degree(gg,mode="total"))
    return(aux)
  )

names(compo_list)=list_names
n=max(sapply(compo_list,FUN=function(x) {length(x[[1]])}))
n

[1] 234

size_compo_list=lapply(compo_list,FUN=function(x) {
  return(c(x[[1]],rep(NA,n-length(x[[1]]))))}

aux=do.call(bind_cols,size_compo_list)
aux2=pivot_longer(aux,aaf:zvi,names_to="Organism",
                  values_to="csize") %>%
  arrange(Organism,-csize)
aux2$index=rep(1:n,times=dim(aux)[2])
aux2=aux2 %>%
  left_join(meta_taxo,by="Organism")

Organism=names(compo_list)
big_MBB=function(org){
  x=Results %>% filter(Organism==org)
  x=as.character(x[1,5:dim(Results)[2]])
  x=x[x!="NA"]
  tt=sort(table(x),decreasing=TRUE)
  return(tt)
}
big_MBB_list= lapply(Organism,FUN=function(x) big_MBB(x))
nMBB=max(sapply(big_MBB_list,FUN=function(x) length(x)))
nMBB

[1] 1042

big_MBB_list=lapply(big_MBB_list,
                     FUN=function(x){
  x=c(x,rep(NA,nMBB-length(x)))
  return(x)}
)
names(big_MBB_list)=Organism

```

```

big_MBB_list=do.call(bind_cols,big_MBB_list)

kMBB=nrow(big_MBB_list)
index=rep(1:kMBB,times=length(Organism))

big_MBB_list2=pivot_longer(big_MBB_list,
                           cols=names(big_MBB_list),
                           values_to = "MBBszie",
                           names_to = "Organism") %>%
  arrange(Organism,-MBBszie) %>%
  mutate(index=index) %>%
  left_join(meta_taxo,by="Organism")

```

5.2.1 Sizes of MBB for each mDAG

```

COLOR_KINGDOM=c("red","green","yellow","black")
colors_kingdom=big_MBB_list2 %>%
  select(Organism,Kingdom) %>%
  distinct()

names(COLOR_KINGDOM)=sort(unique(colors_kingdom$Kingdom))

p0<-ggplot(data=big_MBB_list2) +
  geom_line(mapping=aes(x=index,
                        y=MBBszie,
                        group = Organism,
                        color=Kingdom)) +
  scale_y_continuous(trans='log10') +
  scale_x_continuous(trans='identity') +
  scale_color_manual(values =COLOR_KINGDOM[colors_kingdom$Kingdom]) +
  ggtitle("Plot log-identity of MBB \n decreasing index.") +
  ylab("Log10 MBB size") + xlab("Index")

p1<- ggplot(data=big_MBB_list2) +
  geom_line(mapping=aes(x=index,
                        y=MBBszie,
                        group = Organism,color=Kingdom),
            na.rm=TRUE) +
  scale_x_continuous(trans='log10') +
  scale_y_continuous(trans='log10') +
  scale_color_manual(values =COLOR_KINGDOM[colors_kingdom$Kingdom]) +

```

```

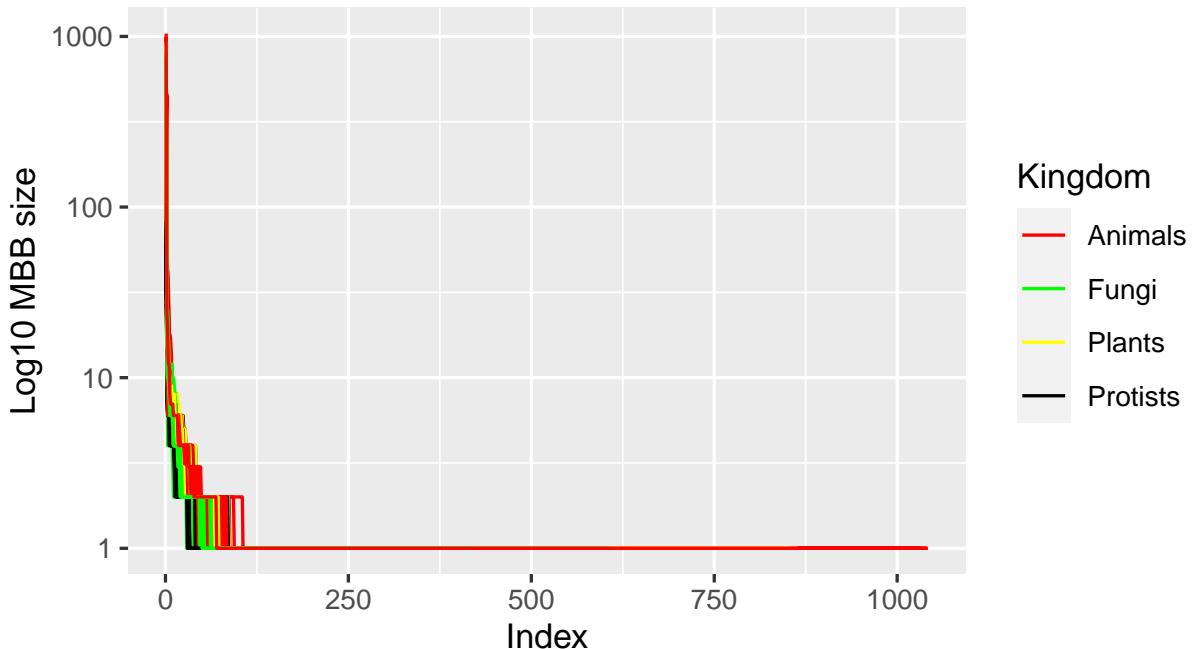
ggttitle("Plot log10-log10identity of MBB \n decreasing index.") +
ylab("Log10 MBB size") + xlab("Log10 Index")

p2<- ggplot(data=big_MBB_list2) +
  geom_line(mapping=aes(x=index,
                        y=MBBsize,
                        group = Organism,
                        color=Kingdom),
            na.rm=TRUE)+ 
  scale_x_continuous(trans="identity") +
  scale_y_continuous(trans="identity") +
  ylim(0,1039) +
  ggttitle("Plot of MBB sized decreasing index.") +
  ylab("MBB size") + xlab("Index") +
  scale_color_manual(values =COLOR_KINGDOM[colors_kingdom$Kingdom])

```

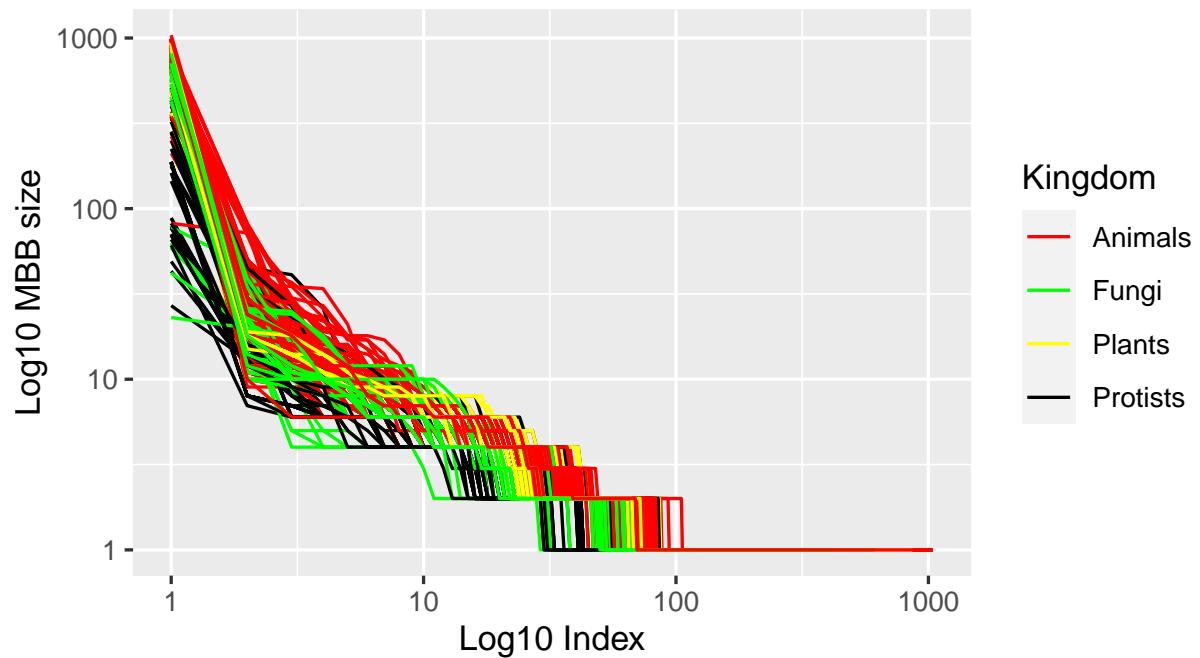
p0

Plot log–identity of MBB decreasing index.



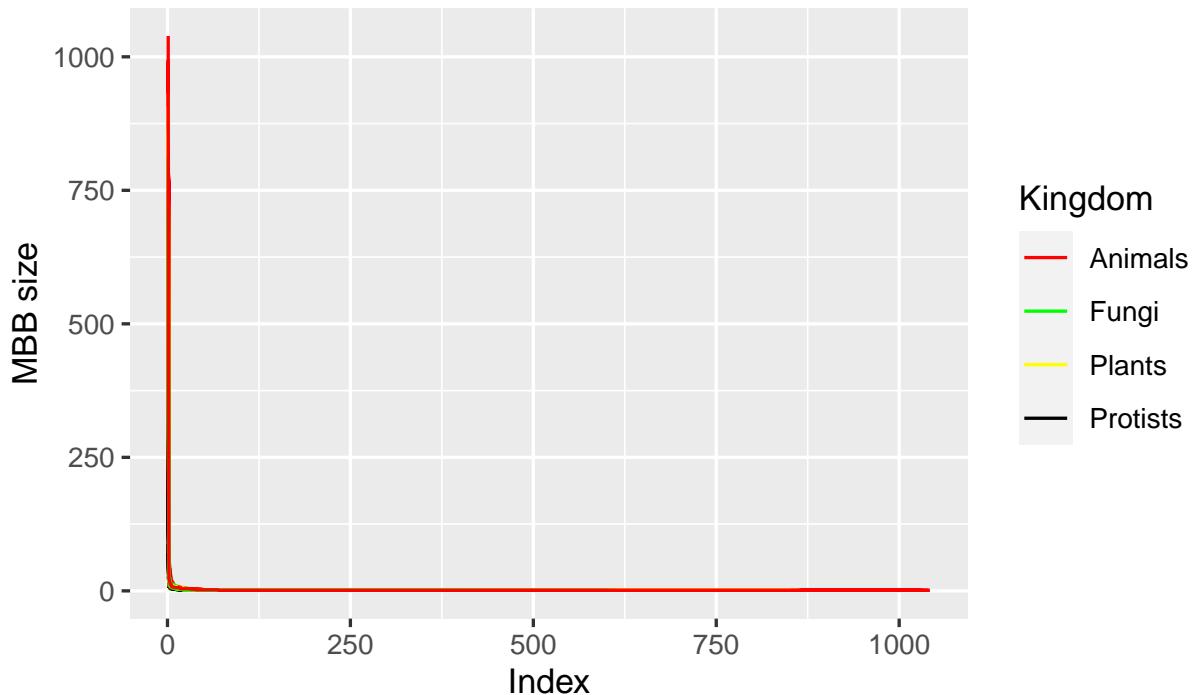
p1

Plot log10–log10identity of MBB
decreasing index.



p2

Plot of MBB sized decreasing index.



5.2.2 Sizes of weak components for each mDAG

```
COLOR_KINGDOM=c("red","yellow","green","yellow","black")
colors_kingdom=aux2%>% select(Organism,Kingdom) %>% distinct()
names(COLOR_KINGDOM)=sort(unique(colors_kingdom$Kingdom))

p0<-ggplot(data=aux2) +
  geom_line(mapping=aes(x=index,
                        y=csizes,
                        group = Organism,
                        color=Kingdom),
            na.rm=TRUE) +
  scale_x_continuous(trans='log10') +
  scale_y_continuous(trans='identity') +
  scale_color_manual(values =COLOR_KINGDOM[colors_kingdom$Kingdom]) +
  ggtitle("Plot log-identity of size weak components decreasing index.") +
  ylab("Log10 Weak componente size") + xlab("Index")

p1<- ggplot(data=aux2) +
```

```

geom_line(mapping=aes(x=index,
                      y=csize, group = Organism,
                      color=Kingdom),
          na.rm=TRUE) +
scale_y_continuous(trans='log10') +
scale_x_continuous(trans='log10') +
scale_color_manual(values =COLOR_KINGDOM[colors_kingdom$Kingdom])+  

  ggtitle("Plot log-log of size weak components decreasing index.") +
  ylab("Log10 weak component size") + xlab("Log10 Index")

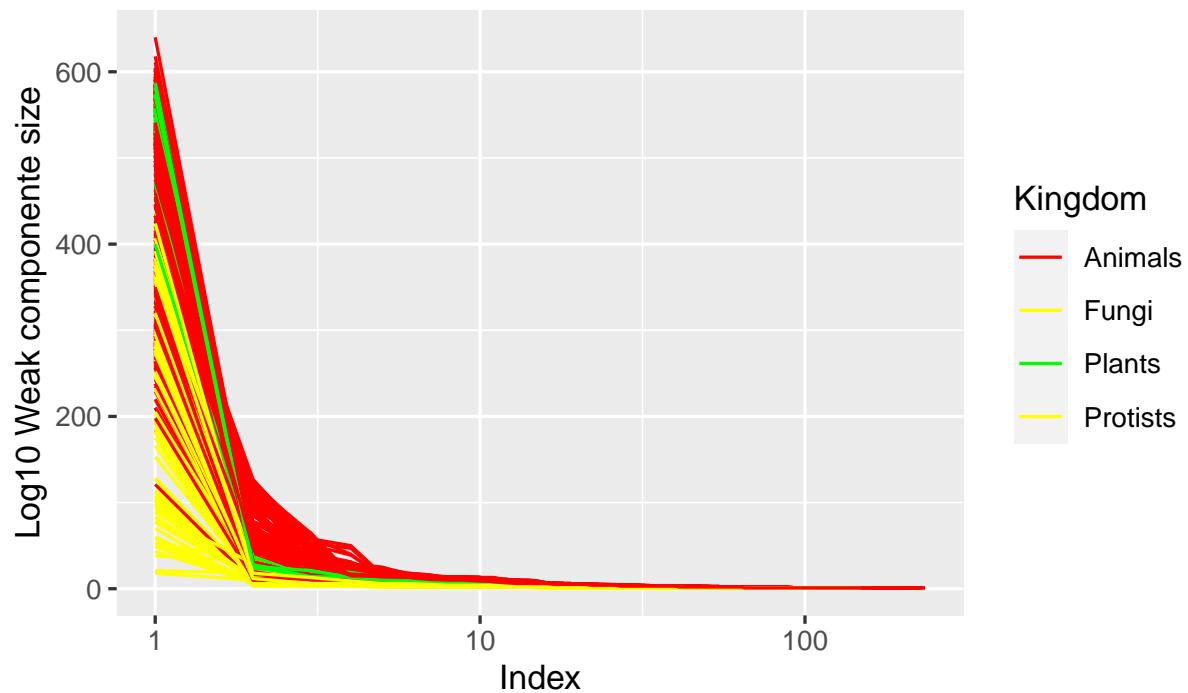
p2<- ggplot(data=aux2) +
  geom_line(mapping=aes(x=index,
                        y=csize, group = Organism,
                        color=Kingdom),
            na.rm=TRUE) +
  scale_x_continuous(trans="identity") +
  scale_y_continuous(trans="identity") +
  ylim(0,1039)+  

  ggtitle("Plot of size weak components decreasing index.")+
  ylab("Weak components size") + xlab("Index")+
  scale_color_manual(values =COLOR_KINGDOM[colors_kingdom$Kingdom])

```

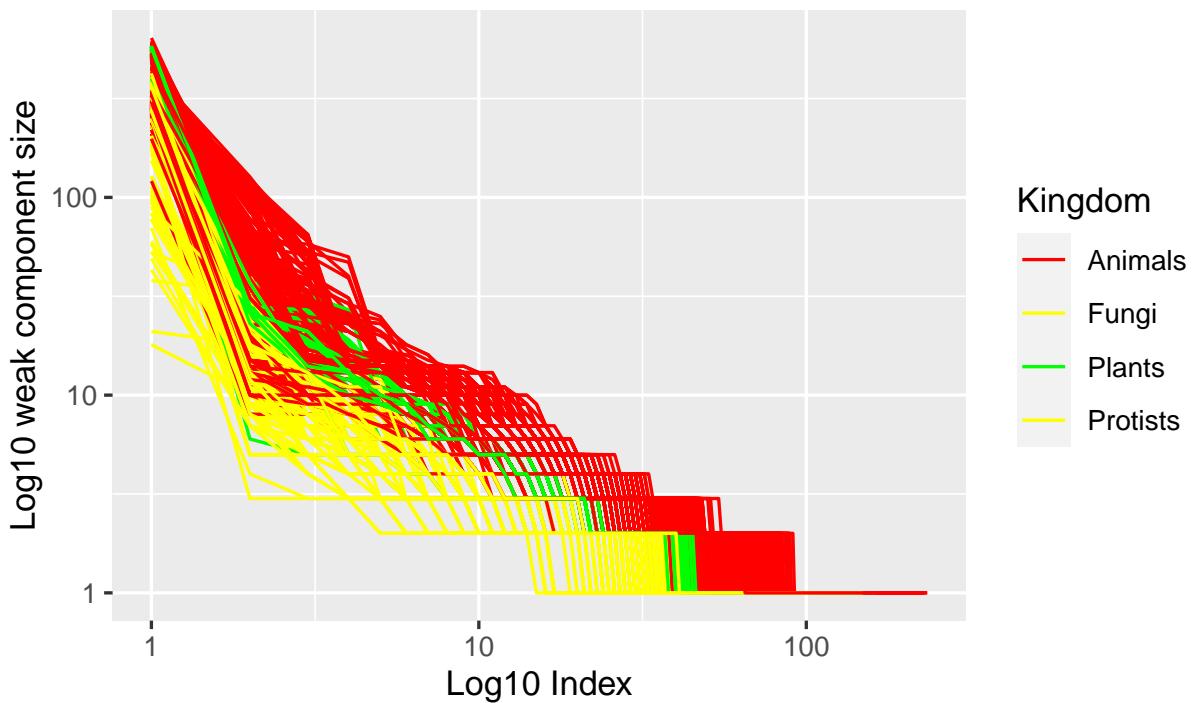
p0

Plot log–identity of size weak components decreasing index.



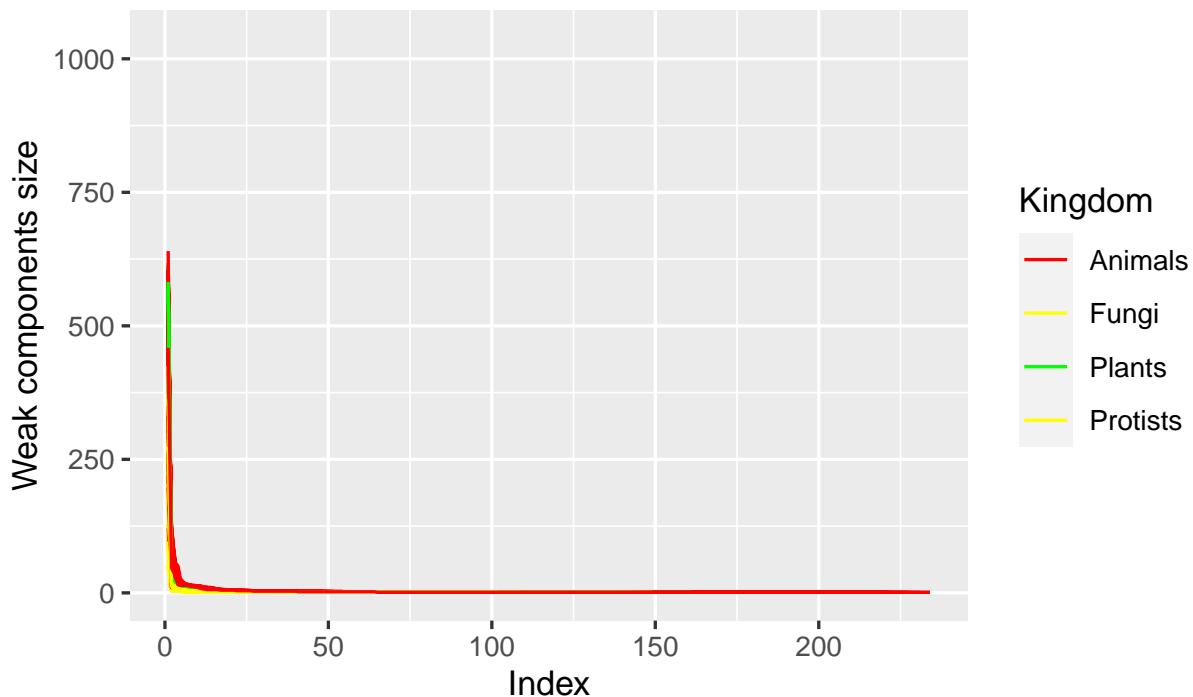
p1

Plot log–log of size weak components decreasing index.



p2

Plot of size weak components decreasing index.



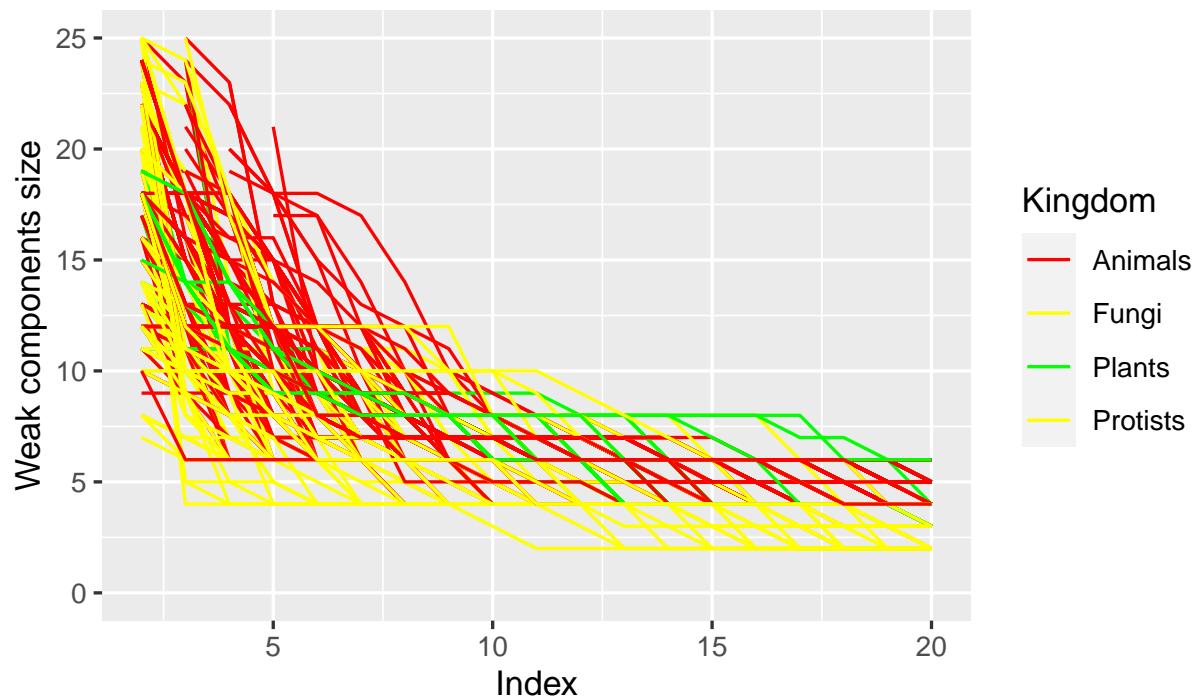
```

data2=big_MBB_list2 %>% filter(index %in% 2:20)
p3<- ggplot(data=data2) +
  geom_line(mapping=aes(x=index,
                        y=MBBsize,
                        group = Organism,
                        color=Kingdom),
            na.rm=TRUE) +
  scale_x_continuous(trans="identity") +
  scale_y_continuous(trans="identity") +
  ylim(0,25) +
  ggtitle("Plot of size weak components decreasing index 2 to 20.") +
  ylab("Weak components size") + xlab("Index") +
  scale_color_manual(values =COLOR_KINGDOM[colors_kingdom$Kingdom])

```

p3

Plot of size weak components decreasing index 2 to 20.



6 Comparison core's all algae, fungi and archaea and clusters

```
reactions=names(Results)[-c(1:4)]
cores=tibble(reactions)
cores=cores %>% separate(reactions, into=c("reactions","enzyme"), sep="\\"(")

cores= cores %>% separate(reactions,into=c("reactions","reactions2"),sep="\\"|",fill = "right")

cores$enzyme=gsub("\\\\(|\\\\)",replacement = "",cores$enzyme)
cores

# A tibble: 3,994 x 3
  reactions reactions2 enzyme
  <chr>     <chr>     <chr>
1 Full_Name <NA>      <NA>
2 R00710    <NA>      1.2.1.3
3 R00710_rev <NA>      1.2.1.3
4 R00711    <NA>      1.2.1.5
5 R00711_rev <NA>      1.2.1.5
6 R00755    <NA>      4.1.1.1
7 R00746    <NA>      1.1.1.2
8 R00746_rev <NA>      1.1.1.2
9 R00754    <NA>      1.1.1.1
10 R00754_rev <NA>      1.1.1.1
# i 3,984 more rows

#algae_core=
```

6.1 Comparison 4 kingdoms and 4 cluster for MSA and Munkrest

```
clust4_MSA2=tibble(mDAG_Id=names(clust4_MSA), clust4_MSA=clust4_MSA)
clust4_Mun2=tibble(mDAG_Id=names(clust4_Mun), clust4_Mun=clust4_Mun)
```

```

meta_taxo2=meta_taxo
meta_taxo2=meta_taxo2 %>% left_join(clust4_MSA2,by= "mDAG_Id") %>%
  left_join(clust4_Mun2,by= "mDAG_Id")
meta_taxo2$combined_cluster_MSA_Kingdom=paste0(meta_taxo2$Kingdom,meta_taxo2$clust4_MSA)
meta_taxo2$combined_cluster_Mun_Kingdom=paste0(meta_taxo2$Kingdom,meta_taxo2$clust4_MSA)
write.csv(meta_taxo2,file="meta_taxo_4_clusters.csv")

knitr::kable(table(meta_taxo2$Kingdom,meta_taxo2$clust4_MSA))



|          | 1   | 2   | 3   | 4   |
|----------|-----|-----|-----|-----|
| Animals  | 331 | 197 | 7   | 0   |
| Fungi    | 0   | 0   | 154 | 0   |
| Plants   | 0   | 0   | 14  | 125 |
| Protists | 0   | 0   | 56  | 0   |



knitr::kable(table(meta_taxo2$Kingdom,meta_taxo2$clust4_Mun))



|          | 1   | 2   | 3   | 4   |
|----------|-----|-----|-----|-----|
| Animals  | 331 | 197 | 7   | 0   |
| Fungi    | 0   | 0   | 154 | 0   |
| Plants   | 0   | 0   | 14  | 125 |
| Protists | 0   | 0   | 56  | 0   |



knitr::kable(table(meta_taxo2$clust4_Mun,meta_taxo2$clust4_MSA))



| 1   | 2   | 3   | 4   |
|-----|-----|-----|-----|
| 331 | 0   | 0   | 0   |
| 0   | 197 | 0   | 0   |
| 0   | 0   | 231 | 0   |
| 0   | 0   | 0   | 125 |



library(reshape2)
MSA_table=melt(table(meta_taxo2$Kingdom,meta_taxo2$Phylum,meta_taxo2$clust4_MSA))
names(MSA_table)=c("Kingdom","Phylum","cluster_MSA","N")
MSA_table=MSA_table %>% filter(N!=0)

knitr::kable(MSA_table)

```

Kingdom	Phylum	cluster_MSA	N
Animals	Vertebrates	1	331
Animals	Annelids	2	1
Animals	Arthropods	2	158
Animals	Brachiopodas	2	1
Animals	Cephalochordates	2	2
Animals	Cnidarians	2	10
Animals	Echinoderms	2	3
Animals	Hemichordates	2	1
Animals	Mollusks	2	14
Animals	Nematodes	2	3
Animals	Placozoans	2	1
Animals	Poriferans	2	1
Animals	Tunicates	2	2
Protists	Alveolates	3	25
Protists	Amoebozoa	3	7
Fungi	Ascomycetes	3	113
Fungi	Basidiomycetes	3	36
Protists	Choanoflagellates	3	2
Protists	Cryptomonads	3	1
Protists	Euglenozoa	3	9
Animals	Flatworms	3	4
Plants	Green	3	11
Protists	Haptophyta	3	1
Protists	Heterolobosea	3	1
Protists	Metamonada	3	2
Fungi	Microsporidians	3	5
Animals	Nematodes	3	3
Plants	Red	3	3
Protists	Stramenopiles	3	8
Plants	Basal	4	2
Plants	Eudicots	4	98
Plants	Ferns	4	1
Plants	Monocots	4	23
Plants	Mosses	4	1

6.2 Comparison core's all algae, fungi and archaea

```
reactions=names(Results)[-c(1:5)]
cores=tibble(reactions)
```

```

cores=cores %>% separate(reactions, into=c("reactions", "enzyme"), sep="\\\\(")

#cores= cores %>% separate(reactions,into=c("reactions", "reactions2"),sep="\\"/,fill = "right"

cores$enzyme=gsub("\\\\(|\\\\)",replacement = "",cores$enzyme)
cores

# A tibble: 3,993 x 2
  reactions   enzyme
  <chr>        <chr>
1 R00710      1.2.1.3
2 R00710_rev  1.2.1.3
3 R00711      1.2.1.5
4 R00711_rev  1.2.1.5
5 R00755      4.1.1.1
6 R00746      1.1.1.2
7 R00746_rev  1.1.1.2
8 R00754      1.1.1.1
9 R00754_rev  1.1.1.1
10 R00014     4.1.1.1
# i 3,983 more rows

#algae_core=

#Results
#cores
#meta_taxo
cores_names=unique(Results$Groups)
cores_names

[1] "MSA Cluster 3|MUN Cluster 3"
[2] "MSA Cluster 2|MUN Cluster 2"
[3] "Fungui and Algae|MSA Cluster 3|MSA Fungui and Nematodes and Flatworms|MUN Cluster 3|MUN
[4] "Cluster 1"
[5] "Cluster 4"
[6] "Algae|Fungui and Algae|MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MUN Algae and
[7] "MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and Nematodes and Flatwo
[8] "MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and Nematodes and Flatwo
[9] "MSA Cluster 2|MUN Cluster 2|whole set of worms"

cores_combi=function(x){
#x=cores_names[1]

```

```

Id=meta_taxo2 %>% filter(Groups==x) %>% select(mDAG_Id)
Id=as.character(Id$mDAG_Id)
#bin_NA=function(x) {case_when(!is.na(x) ~ 0 , default=1)}
not_NA= function(x) {!is.na(x)}

mda_filter= Results %>%
  filter(mDAG_Id %in% Id) %>%
  select(starts_with("R")) %>%
  mutate_all(not_NA) %>% mutate_all(as.integer)

#%>%
#  mutate(mDag_id=Id,.before=1)
#aux=colSums(mda_filter)
#aux=as.integer(aux==length(Id))
return(mda_filter)
}

cores_list=lapply(cores_names,cores_combi)
lapply(cores_list,dim)

[[1]]
[1] 56 3993

[[2]]
[1] 194 3993

[[3]]
[1] 154 3993

[[4]]
[1] 331 3993

[[5]]
[1] 125 3993

[[6]]
[1] 14 3993

[[7]]
[1] 7 3993

[[8]]

```

```

[1] 2 3993

[[9]]
[1] 1 3993

cores_raw=lapply(cores_list,FUN=function(X){apply(X,2,prod)})

aux=cores_raw %>% as_tibble(.name_repair ="universal")
names(aux)=cores_names
cores = cbind(cores,aux)

names(cores)

[1] "reactions"
[2] "enzyme"
[3] "MSA Cluster 3|MUN Cluster 3"
[4] "MSA Cluster 2|MUN Cluster 2"
[5] "Fungui and Algae|MSA Cluster 3|MSA Fungui and Nematodes and Flatworms|MUN Cluster 3|MUN
[6] "Cluster 1"
[7] "Cluster 4"
[8] "Algae|Fungui and Algae|MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MUN Algae and
[9] "MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and Nematodes and Flatw
[10] "MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and Nematodes and Flatw
[11] "MSA Cluster 2|MUN Cluster 2|whole set of worms"

knitr::kable(colSums(cores[,-c(1,2)]),col.names = c("Freq"))



---


MSA Cluster 3|MUN Cluster 3
MSA Cluster 2|MUN Cluster 2
Fungui and Algae|MSA Cluster 3|MSA Fungui and Nematodes and Flatworms|MUN Cluster 3|MUN Fungui
Cluster 1
Cluster 4
Algae|Fungui and Algae|MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MUN Algae and Nematodes
MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and Nematodes and Flatworms|MSA
MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and Nematodes and Flatworms|MSA
MSA Cluster 2|MUN Cluster 2|whole set of worms

cores %>% select(reactions,enzyme,`Cluster 1`) %>%
  filter(`Cluster 1`==1) %>%
  mutate(http=paste0("https://www.genome.jp/entry/",reactions))-> pp

knitr::kable(pp)

```

reactions	enzyme
R00710	1.2.1.3
R00710_rev	1.2.1.3
R00014	1.2.4.1
R03270	1.2.4.1
R00703	1.1.1.27
R00703_rev	1.1.1.27
R00200	2.7.1.40
R00658	4.2.1.11
R00658_rev	4.2.1.11
R01518	5.4.2.11
R01518_rev	5.4.2.11
R01070	4.1.2.13
R01070_rev	4.1.2.13
R04779	2.7.1.11
R04780	3.1.3.11
R00959	5.4.2.2
R00959_rev	5.4.2.2
R01600	2.7.1.1
R01786	2.7.1.1
R01788	3.1.3.9
R00431 R00726	4.1.1.32
R00235	6.2.1.1
R00621	1.2.4.2
R03316	1.2.4.2
R02570	2.3.1.61
R02570_rev	2.3.1.61
R00405	6.2.1.5
R00405_rev	6.2.1.5
R00432 R00727	6.2.1.4
R00432 R00727_rev	6.2.1.4
R00268	1.1.1.42
R00268_rev	1.1.1.42
R00709	1.1.1.41
R00709_rev	1.1.1.41
R01899	1.1.1.42
R01899_rev	1.1.1.42
R00352	2.3.3.8
R00352_rev	2.3.3.8
R02164	1.3.5.1
R02164_rev	1.3.5.1
R01900	4.2.1.3
R01900_rev	4.2.1.3
R01325	4.2.1.3
R01325_rev	4.2.1.39
R00342	1.1.1.37
R00342_rev	1.1.1.37
R01641	2.2.1.1
R01641_rev	2.2.1.1
R01830	2.2.1.1
R01830_rev	2.2.1.1
R01057	5.4.2.2

```
cores %>%
  select(reactions,enzyme,`Algae|Fungui and Algae|MSA Algae and Nematodes and Flatworms|MSA`)
  filter(`Algae|Fungui and Algae|MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MUN Alga`)
  mutate(http=paste0\("https://www.genome.jp/entry/",reactions\)\)-> pp
knitr::kable(pp)
```

reactions	enzyme
R00754	1.1.1.1
R00754_rev	1.1.1.1
R00014	1.2.4.1
R03270	1.2.4.1
R02569	2.3.1.12
R02569_rev	2.3.1.12
R00200	2.7.1.40
R00658	4.2.1.11
R00658_rev	4.2.1.11
R01015	5.3.1.1
R01015_rev	5.3.1.1
R01070	4.1.2.13
R01070_rev	4.1.2.13
R04779	2.7.1.11
R04780	3.1.3.11
R02740	5.3.1.9
R02740_rev	5.3.1.9
R00959	5.4.2.2
R00959_rev	5.4.2.2
R03321	5.3.1.9
R03321_rev	5.3.1.9
R02739	5.3.1.9
R02739_rev	5.3.1.9
R02739	5.1.3.15
R02739_rev	5.1.3.15
R01512	2.7.2.3
R01512_rev	2.7.2.3
R00235	6.2.1.1
R00405	6.2.1.5
R00405_rev	6.2.1.5
R00432 R00727	6.2.1.4
R00432 R00727_rev	6.2.1.4
R02164	1.3.5.1
R02164_rev	1.3.5.1
R01082	4.2.1.2
R01082_rev	4.2.1.2
R00351	2.3.3.1
R00351_rev	2.3.3.1
R00342	1.1.1.37
R00342_rev	1.1.1.37
R01641	2.2.1.1
R01641_rev	2.2.1.1
R01056	5.3.1.6
R01056_rev	5.3.1.6 ₁
R01529	5.1.3.1
R01529_rev	5.1.3.1
R01830	2.2.1.1
R01830_rev	2.2.1.1
R02035	3.1.1.31
R02736	1.1.1.49
R01057	5.4.2.2

```

cores %>%
  select(reactions,enzyme,"MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and
  filter("MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and Nematodes and F
  mutate(http=paste0("https://www.genome.jp/entry/",reactions))-> pp

knitr::kable(pp)



| reactions | enzyme | MSA Algae and Nematodes and Flatworms MSA Cluster 3 MSA Fungui and Nematode |
|-----------|--------|-----------------------------------------------------------------------------|
|           |        |                                                                             |



cores %>%
  select(reactions,enzyme,"MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and
  filter("MSA Algae and Nematodes and Flatworms|MSA Cluster 3|MSA Fungui and Nematodes and F
  mutate(http=paste0("https://www.genome.jp/entry/",reactions))-> pp

knitr::kable(pp)



| reactions | enzyme | MSA Algae and Nematodes and Flatworms MSA Cluster 3 MSA Fungui and Nematode |
|-----------|--------|-----------------------------------------------------------------------------|
|           |        |                                                                             |


```