

Main class for investigation of metaproteome data

Name: Start.m Author: Robert Heyer Date : 01.06.2015 Version: 03

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Clean everything

```
clc; clear all; close all;
```

Load classifications

C.reactor, C.pH, C.tan, C.power,C.biogas, C.vfa, C.oler, C.srt, C.temp , C.fa, C.biogasPerOlr

```
C = LoadClassification();
```

Taxonomy Data

1. Read taxonomy data

```
[tax_matrix_original, TaxMatrixPlusDescription] = ReadTaxFiles();  
% Sort by taxonomy profile  
  
% 2. Remove root entry  
for root = 1: size(tax_matrix_original, 1)  
    if (strcmp(tax_matrix_original(root,1), 'root'))  
        tax_matrix_original(root,:) = [];  
        break  
    end  
end  
clearvars root;  
  
% 3. Contracting the length of the sample names  
for entry = 2: size(tax_matrix_original, 2)  
    str = cell2mat(tax_matrix_original(1, entry));  
    tax_matrix_original(1, entry) = {regexprep(str, 'RH_Tax_Order_UniRef50_allSpecies_Gent', '' )};  
end  
clearvars str, entry;  
  
% Remove "Unknown"-entry  
for unknown = 1: size(tax_matrix_original, 1)  
    if (strcmp(tax_matrix_original(unknown,1), 'unknown'))  
        tax_matrix_original(unknown,:) = [];  
        break; % 'UNKNOWN' is only once in the dataset  
    end  
end  
clearvars unknown;
```

```

end
clearvars unknown;

% 4. Filtering and normalizing of the "tax_matrix_original" with at least
% one entry, were the taxonomy represents at least 1% of the spectra
[tax_matrix_filtered, specAverageBgp] = FilterAndNormalize(tax_matrix_original, 0.01);
% 4b. Sort after the taxTree
tax_matrix_filtered_desc = cell(size(tax_matrix_filtered,1), size(tax_matrix_filtered,2)+5);
tax_matrix_filtered_desc(:,1) = tax_matrix_filtered(:,1);
tax_matrix_filtered_desc(:,7:end) = tax_matrix_filtered(:,2:end);
% Add description to the taxonomy matrix
for tax = 1: size(tax_matrix_filtered,1)
    for entries = 1 : size(TaxMatrixPlusDescription, 1)
        if (isequal(tax_matrix_filtered(tax,1), TaxMatrixPlusDescription(entries,1)) )
            tax_matrix_filtered_desc(tax,2) = TaxMatrixPlusDescription(entries,2); % Superking
            tax_matrix_filtered_desc(tax,3) = TaxMatrixPlusDescription(entries,3); % Kingdom
            tax_matrix_filtered_desc(tax,4) = TaxMatrixPlusDescription(entries,4); % Phylum
            tax_matrix_filtered_desc(tax,5) = TaxMatrixPlusDescription(entries,5); % Class
            tax_matrix_filtered_desc(tax,6) = TaxMatrixPlusDescription(entries,6); % Order
        end
    end
end
clearvars tax entries;

[tax_average_matrix_filtered]= AverageMatrix(tax_matrix_filtered);
% 5. Create the correlation matrix
[tax_correlationMatrix2, pValues] = CalculateCorrelation_V2(tax_average_matrix_filtered, tax_
% Add description to the correlation matrix
tax_correlationMatrix_desc = cell(size(tax_correlationMatrix2,1), size(tax_correlationMatrix2
tax_correlationMatrix_desc(:,1:6) = tax_matrix_filtered_desc(:,1:6);
tax_correlationMatrix_desc(:,7:end) = tax_correlationMatrix2(:,2:end);

% 6. Perform PCA
[coeff, Scores, latent] =PerformPCA(tax_matrix_filtered, tax_matrix_filtered(1, 2:end), 'Tax');
PerformPCA(tax_average_matrix_filtered, tax_average_matrix_filtered(1, 2:end), 'Tax_Norm');

```

```

IMPORTED: RH_Tax_Order_UniRef50_allSpecies_Gent01a
IMPORTED: RH_Tax_Order_UniRef50_allSpecies_Gent01b
IMPORTED: RH_Tax_Order_UniRef50_allSpecies_Gent01c
IMPORTED: RH_Tax_Order_UniRef50_allSpecies_Gent02a
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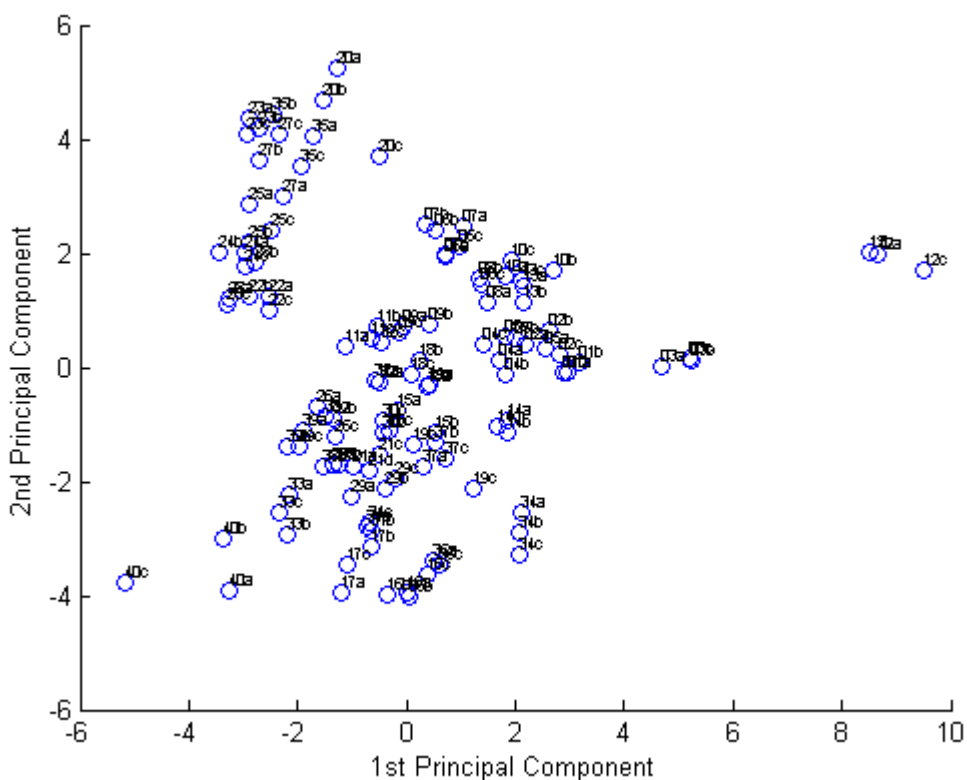
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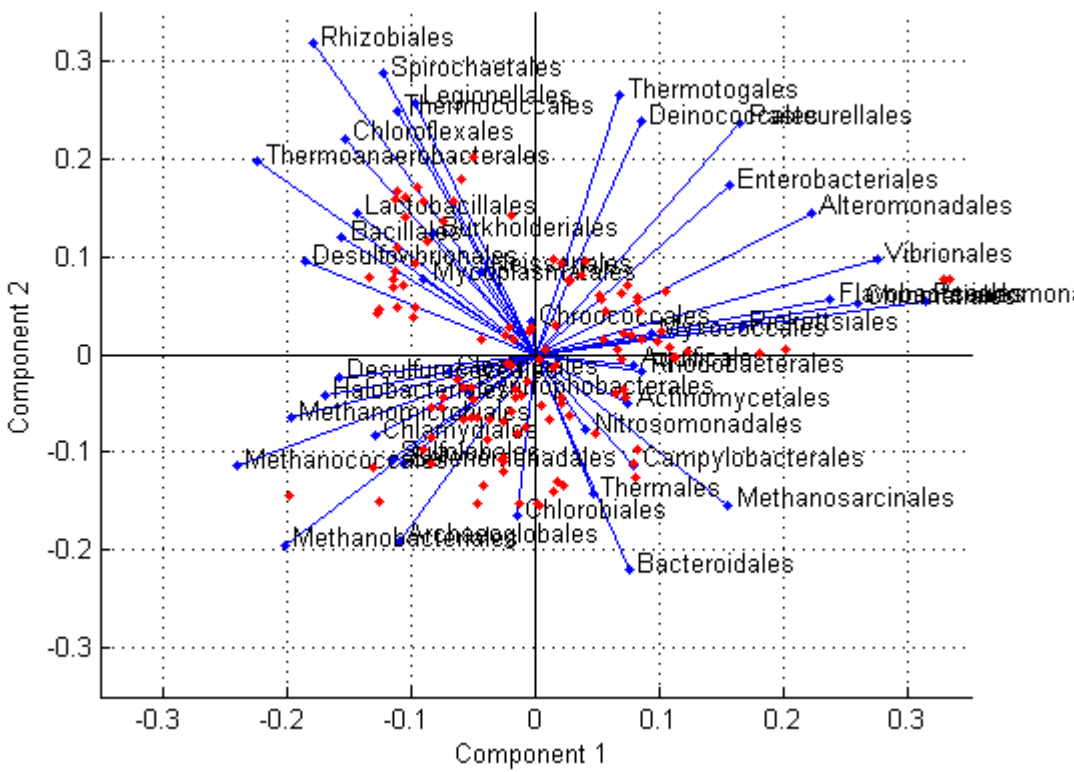
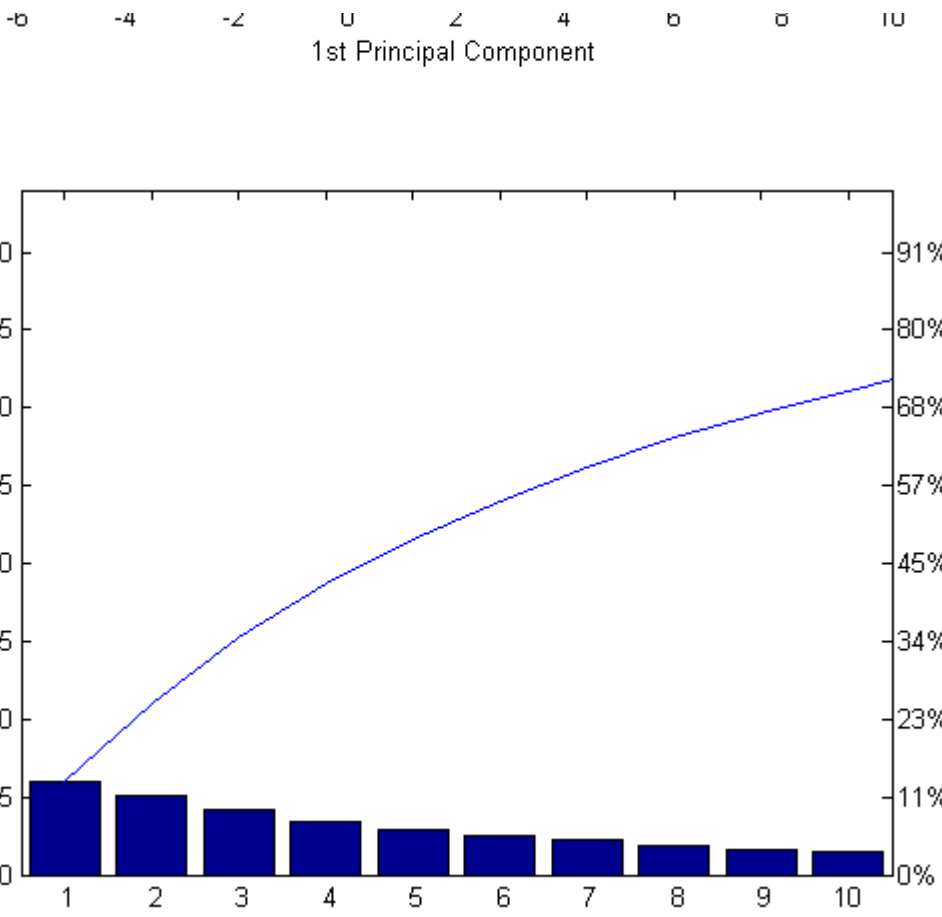
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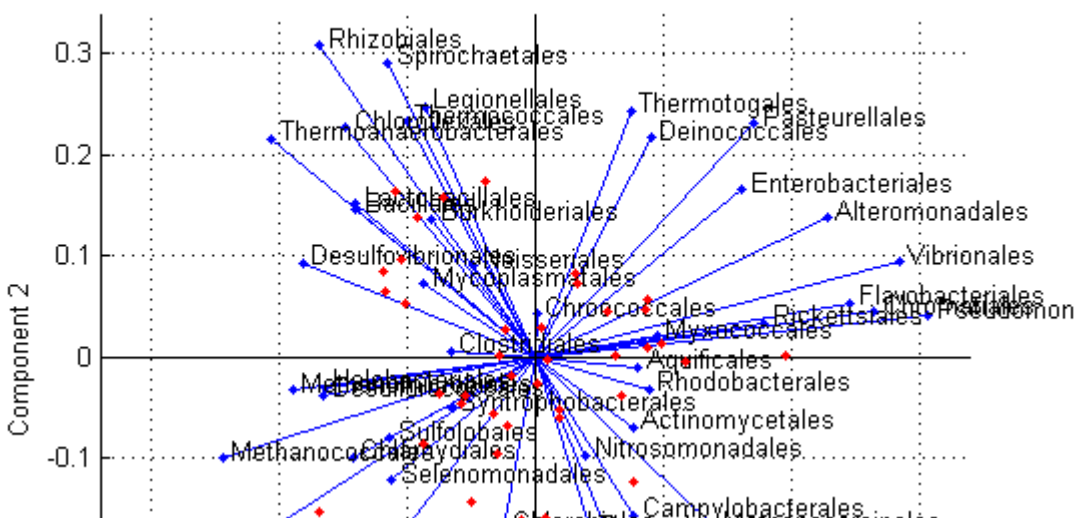
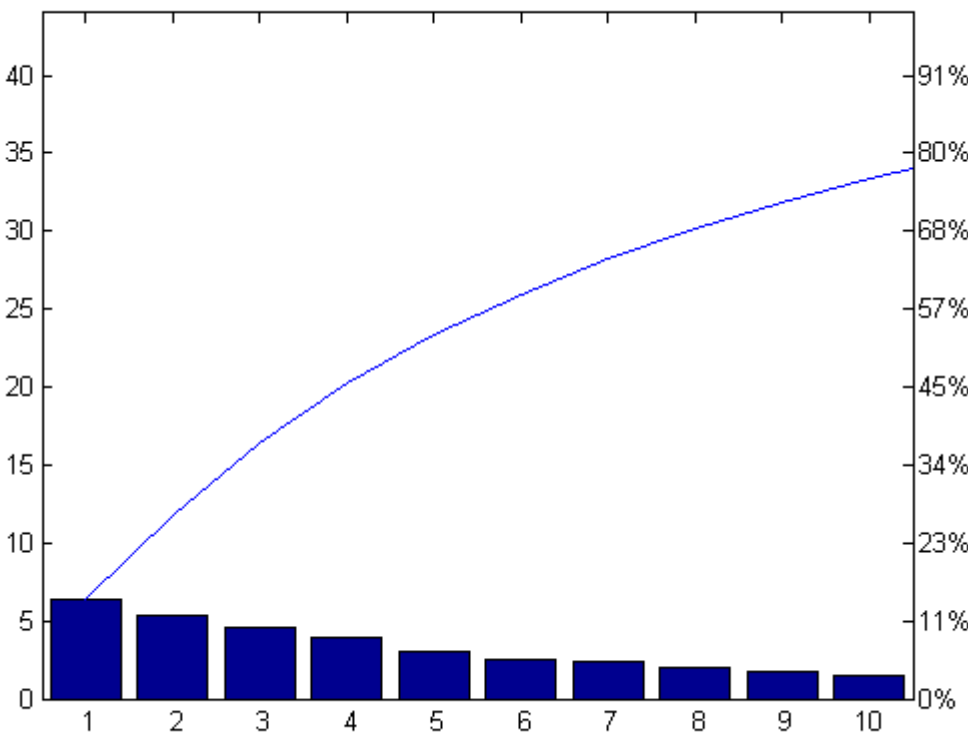
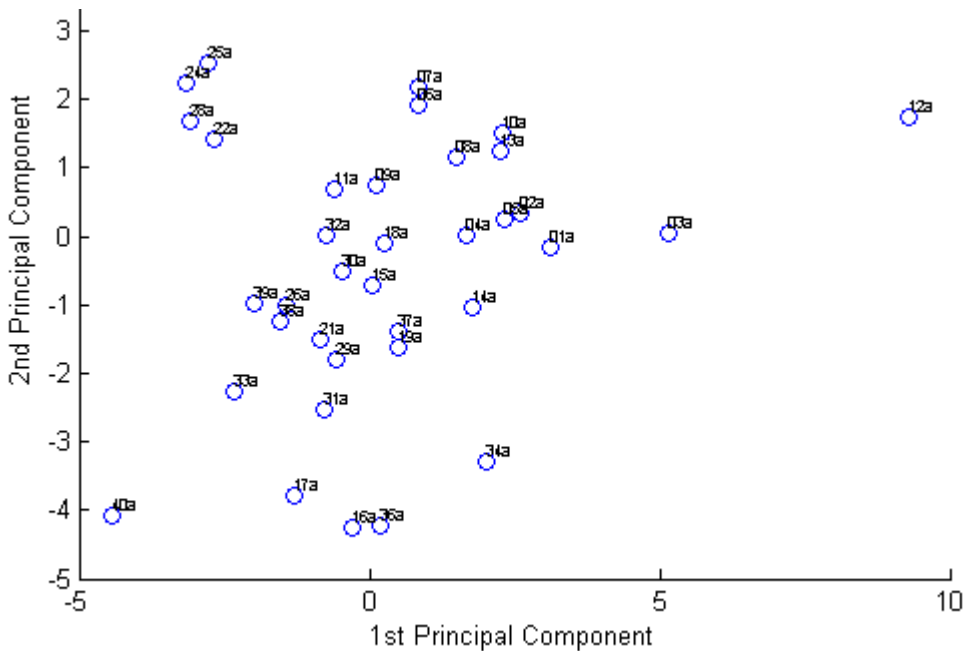
Taxonomy files successfully read:

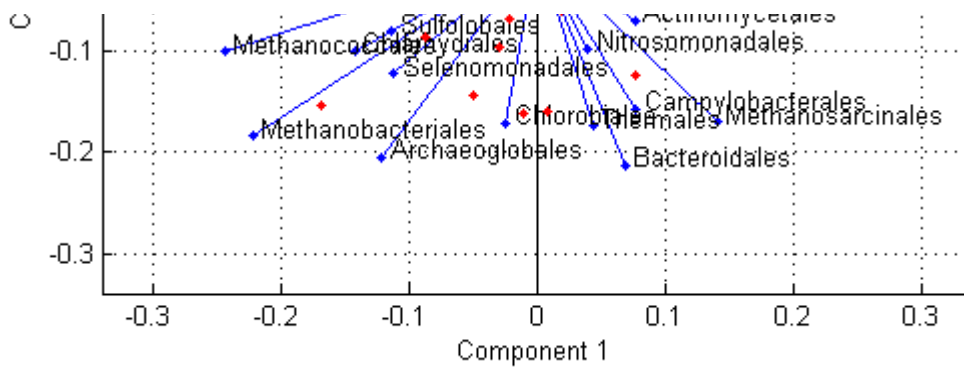
Matrix was normalized and filtered by threshold 0.01 successfully

CrossCorrelation with Spearman matrix successfully calculated









Process data

1. Read process data rows Variables, cols: BGPs (original matrix is transposed)

```
[meta_matrix] = ReadMetaData();

% 3. Calculate Cross Correlations
[meta_correlationMatrix] = CalculateCorrelation_V2(meta_matrix, meta_matrix);
```

CrossCorrelation with Spearman matrix successfully calculated

Biological function Ontology

```
% 1. Read biological functions
[onto_matrix_original] = ReadBiolFunctFiles();

% 2. Shorten the entry in the type list
for entry = 2: size(onto_matrix_original, 2)
    str = cell2mat(onto_matrix_original(1, entry));
    onto_matrix_original(1, entry) = {regexprep(str, 'Gent_onto_BiolFunction_UniRef50_allSpeci
end
clearvars str, entry;

% 3. Filter and normalize the onto_matrix
[onto_matrix_filtered] = FilterAndNormalize(onto_matrix_original, 0.01);

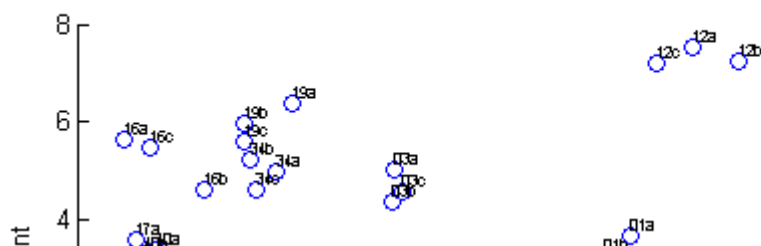
% 4. Create average matrix
[onto_average_matrix_filtered]= AverageMatrix(onto_matrix_filtered);

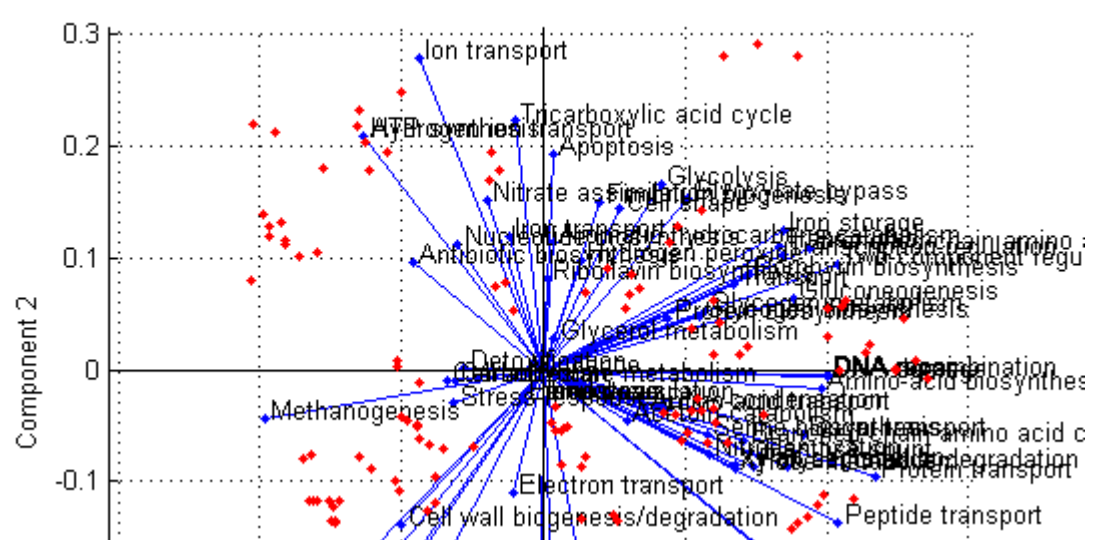
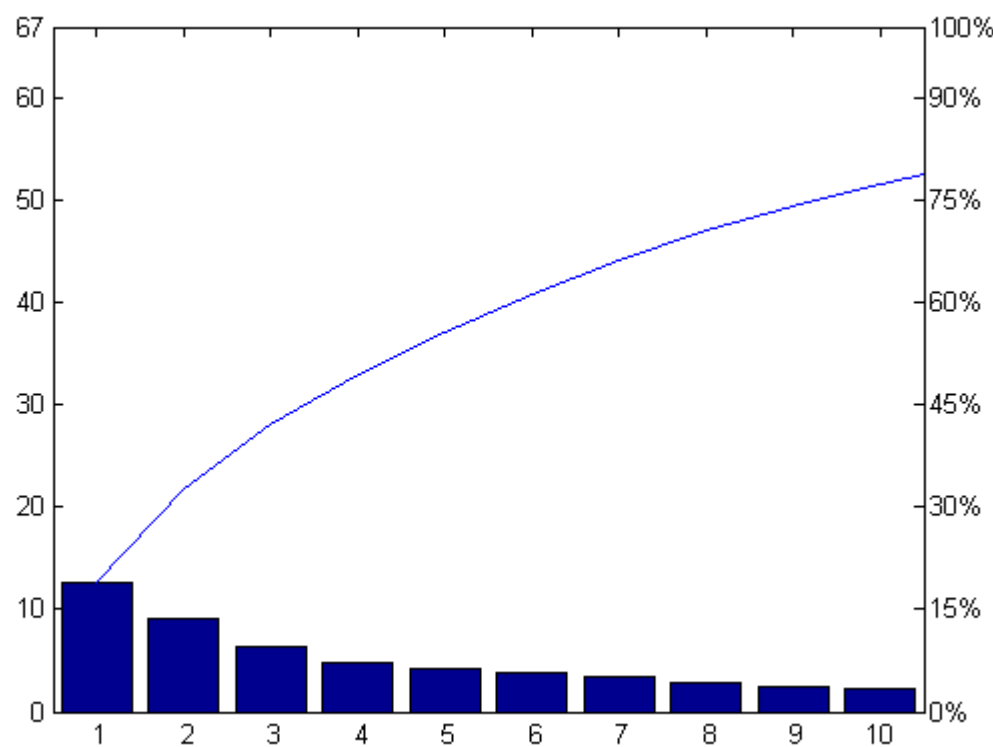
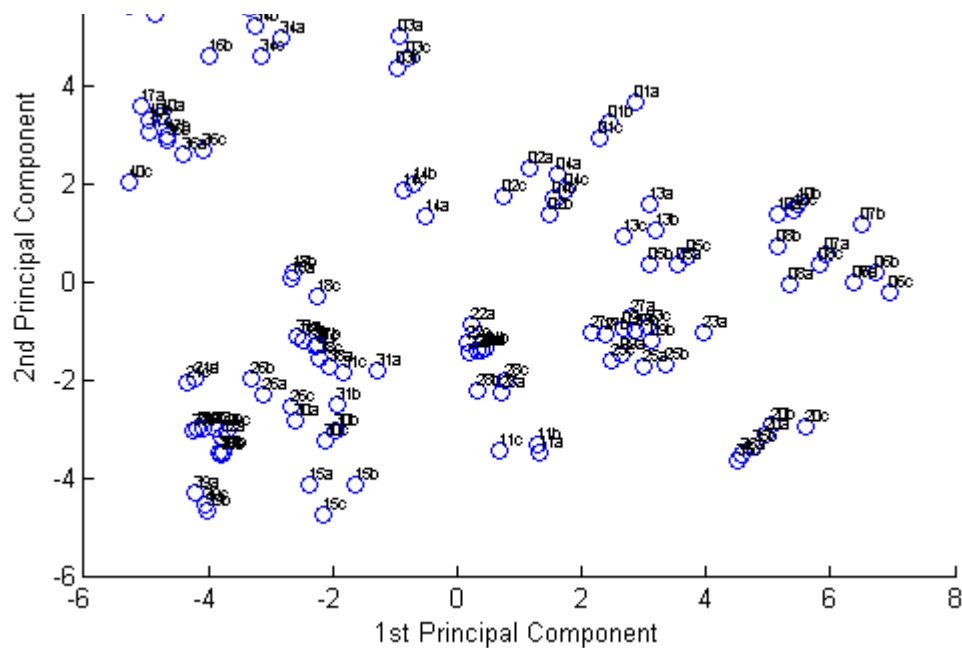
% 5. The correlation matrix
[ onto_correlationMatrix2 ] = CalculateCorrelation_V2(onto_average_matrix_filtered, onto_aver

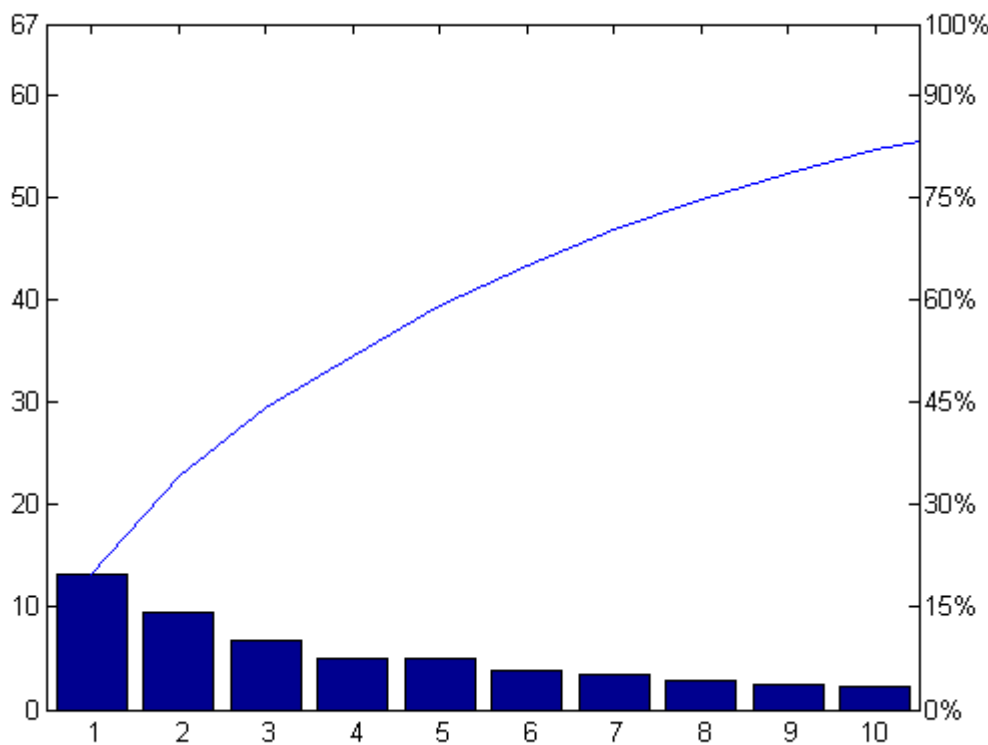
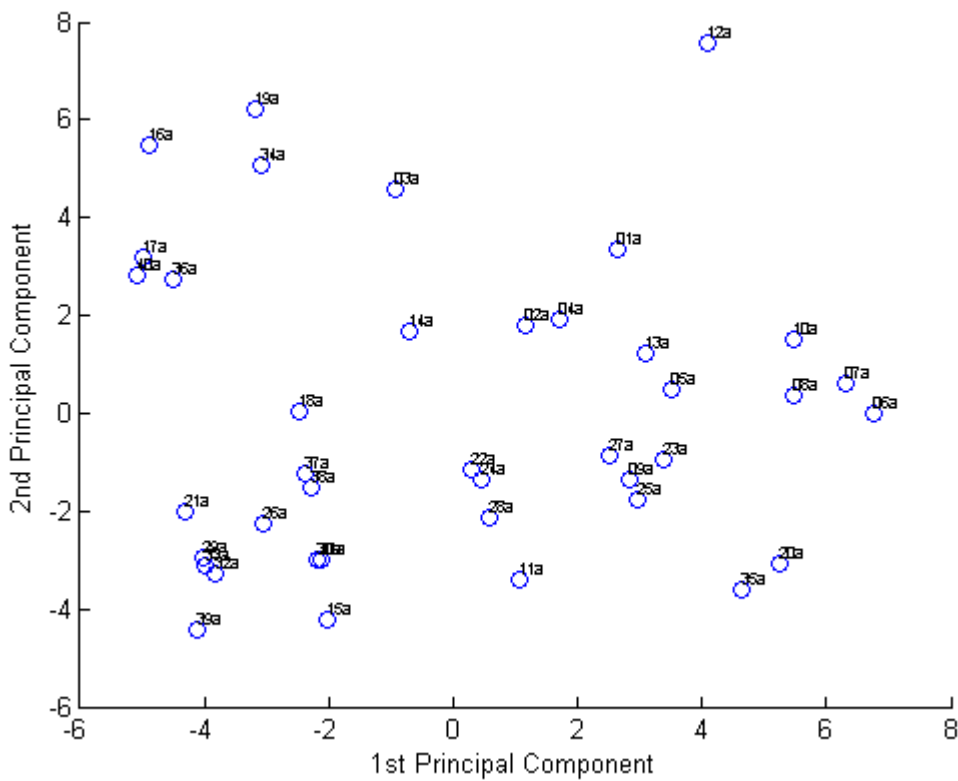
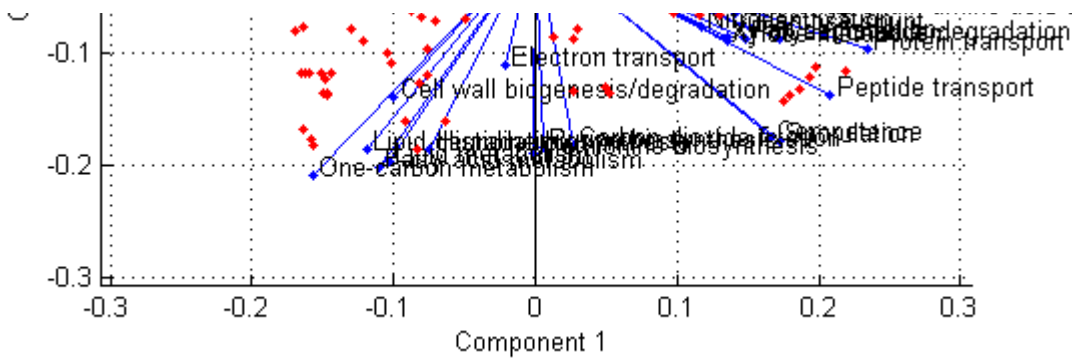
% 6. Perform PCA
[coeff, Scores, latent]= PerformPCA(onto_matrix_filtered, onto_matrix_filtered(1, 2:end), 'Onto_
PerformPCA(onto_average_matrix_filtered, onto_average_matrix_filtered(1, 2:end), 'Onto_Norm');
```

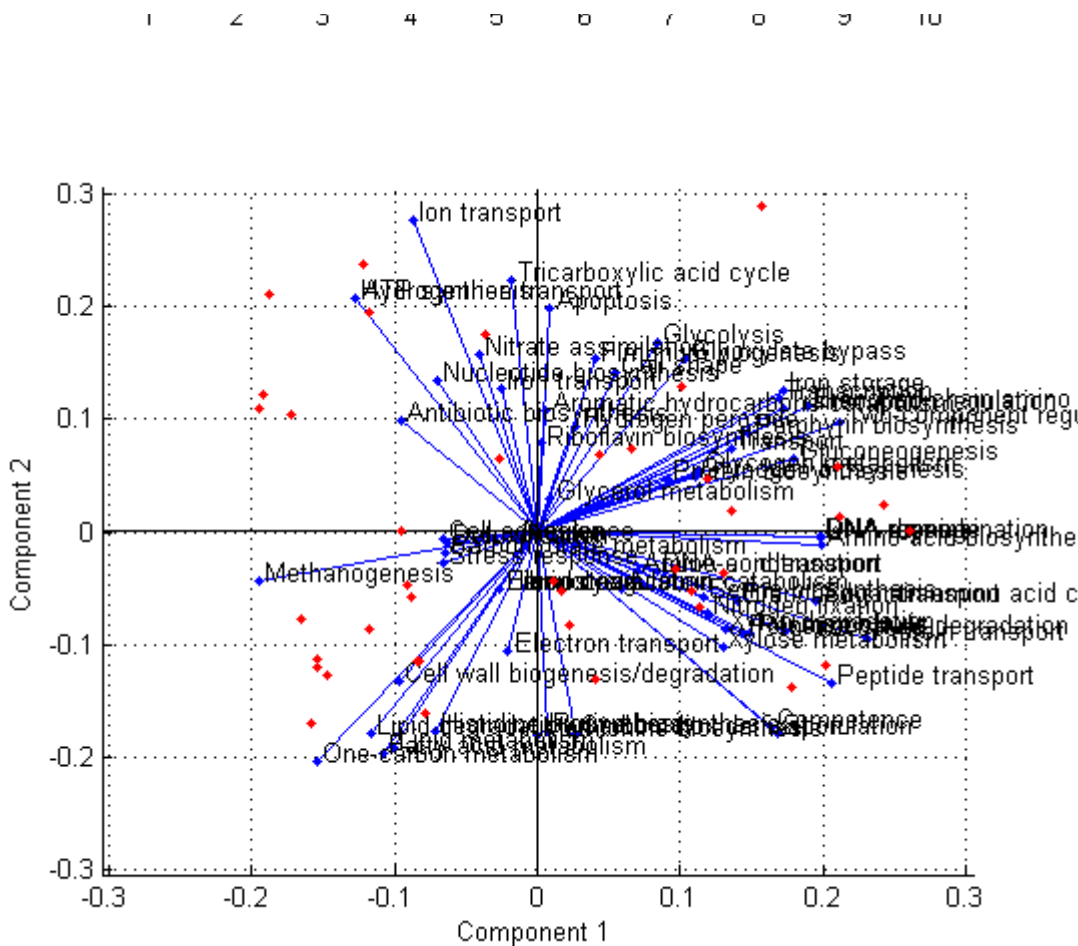
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IMPORTED: Gent_onto_BiolFunction_UniRef50_allSpecies_Gent03c
IMPORTED: Gent_onto_BiolFunction_UniRef50_allSpecies_Gent04a
IMPORTED: Gent_onto_BiolFunction_UniRef50_allSpecies_Gent04b
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IMPORTED: Gent_Onto_BiolFunction_UniRef50_allSpecies_Gent24a
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IMPORTED: Gent_Onto_BiolFunction_UniRef50_allSpecies_Gent40b
IMPORTED: Gent_Onto_BiolFunction_UniRef50_allSpecies_Gent40c
Ontology files successfully read:
Matrix was normalized and filtered by threshold 0.01 successfully
CrossCorrelation with Spearman matrix successfully calculated









Metaprotein Data

```

% 1. Read metaprotein data
[mp_matrix_original, MatrixPlusDescription] = ReadMetaProteinFiles();

% 2. Shorten the entry in the type list and shorten the identifier
for entry = 2: size(mp_matrix_original, 2)
    str = cell2mat(mp_matrix_original(1, entry));
    mp_matrix_original(1, entry) = {regexprep(str, 'Gent_MP_UniRef50_allSpecies_Gent', '')} ;
end
clearvars str entry;

% 3. Remove "Unknown"-entry
for unknown = 1: size(MatrixPlusDescription, 1)
    if (strcmp(MatrixPlusDescription(unknown,1), 'UNKNOWN'))
        mp_matrix_original(unknown,:) = [];
        MatrixPlusDescription(unknown,:) = [];
        break; % 'UNKNOWN' is only once in the dataset
    end
end
clearvars unknown;

% 4. Remove "Keratin"-entries and shorten the identifier
remove = [];
for filtered = 2: size(MatrixPlusDescription, 1)
    if (isempty(strfind(cell2mat(MatrixPlusDescription(filtered,2)), 'Keratin')) == false);
        remove(end+1,1) = filtered;
    end
    % Shorten the identifier by removing UniRef50_
    str = cell2mat(MatrixPlusDescription(filtered,1));
    MatrixPlusDescription(filtered,1) = {regexprep(str, 'UniRef50_', '')};
    mp_matrix_original(filtered,1) = {regexprep(str, 'UniRef50_', '')};
end
remove = sort(remove, 'descend');

```

```

    mp_matrix_original(filtered,1) = {regexprep(str, 'UniRef50_', '')};
end
remove = sort(remove, 'descend');
for r = 1 :length(remove)
    mp_matrix_original(remove(r),:) = [];
    MatrixPlusDescription(remove(r),:) = [];
end
clearvars unknown r remove filtered;

% 5. Filter and normalize the mp_matrix
[mp_matrix_filtered] = FilterAndNormalize(mp_matrix_original, 0.01);
mp_matrix_filtered_desc = cell(size(mp_matrix_filtered,1), size(mp_matrix_filtered,2)+14);
mp_matrix_filtered_desc(:,1) = mp_matrix_filtered(:,1);
mp_matrix_filtered_desc(:,16:end) = mp_matrix_filtered(:,2:end);

% 6. Create average matrix
[mp_average_matrix_filtered]= AverageMatrix(mp_matrix_filtered);
% Add description to the mp_average_matrix
mp_average_matrix_filtered_desc = cell(size(mp_average_matrix_filtered,1), size(mp_average_ma
mp_average_matrix_filtered_desc(:,1) = mp_average_matrix_filtered(:,1);
mp_average_matrix_filtered_desc(:,16:end) = mp_average_matrix_filtered(:,2:end);
% % Add Metainformation
for mp = 2: size(mp_average_matrix_filtered,1)
    for entries = 2 : size(MatrixPlusDescription, 1)
        if (isequal(mp_average_matrix_filtered_desc(mp,1), MatrixPlusDescription(entries,1)) )
            mp_average_matrix_filtered_desc(mp,2) = MatrixPlusDescription(entries,2); % Descri
            mp_average_matrix_filtered_desc(mp,3) = MatrixPlusDescription(entries,3); % Taxonc
            mp_average_matrix_filtered_desc(mp,4) = MatrixPlusDescription(entries,4); % Superk
            mp_average_matrix_filtered_desc(mp,5) = MatrixPlusDescription(entries,5); % Kingdc
            mp_average_matrix_filtered_desc(mp,6) = MatrixPlusDescription(entries,6); % Phylum
            mp_average_matrix_filtered_desc(mp,7) = MatrixPlusDescription(entries,7); % Class
            mp_average_matrix_filtered_desc(mp,8) = MatrixPlusDescription(entries,8); % Order
            mp_average_matrix_filtered_desc(mp,9) = MatrixPlusDescription(entries,9); % Famili
            mp_average_matrix_filtered_desc(mp,10) = MatrixPlusDescription(entries,10); % Genu
            mp_average_matrix_filtered_desc(mp,11) = MatrixPlusDescription(entries,11); % Spec
            mp_average_matrix_filtered_desc(mp,12) = MatrixPlusDescription(entries,12); % UniF
            mp_average_matrix_filtered_desc(mp,13) = MatrixPlusDescription(entries,13); % UniF
            mp_average_matrix_filtered_desc(mp,14) = MatrixPlusDescription(entries,14); % KO
            mp_average_matrix_filtered_desc(mp,15) = MatrixPlusDescription(entries,15); % EC
        end
    end
end
clearvars mp entries;

% 7. The correlation matrix
[ mp_correlationMatrix2 ] = CalculateCorrelation_V2(mp_average_matrix_filtered, mp_average_m
% Add description to the correlation matrix
mp_correlationMatrix2_desc = cell(size(mp_correlationMatrix2,1), size(mp_correlationMatrix2,2
mp_correlationMatrix2_desc(:,1:15) = mp_average_matrix_filtered_desc(:,1:15);
mp_correlationMatrix2_desc(:,16:end) = mp_correlationMatrix2(:,2:end);

% 8. Perform PCA
[coeff,Scores,latent]=PerformPCA(mp_matrix_filtered, mp_matrix_filtered(1, 2:end),'MP_');
PerformPCA(mp_average_matrix_filtered, mp_average_matrix_filtered(1, 2:end),'MP_Norm');

% Perform Clustergram
figure('Name', 'MP:Clustergram');
clustergram(zscore(cell2mat(mp_matrix_filtered(2:end, 2:end))), 'RowLabels', mp_matrix_filt

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IMPORTED: Gent_MP_UniRef50_allSpecies_Gent01a

IMPORTED: Gent_MP_UniRef50_allSpecies_Gent01b

IMPORTED: Gent_MP_UniRef50_allSpecies_Gent01c

IMPORTED: Gent_MP_UniRef50_allSpecies_Gent02a

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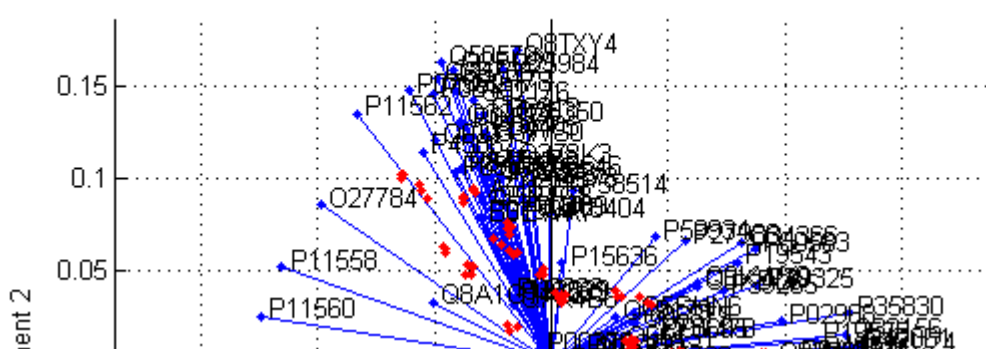
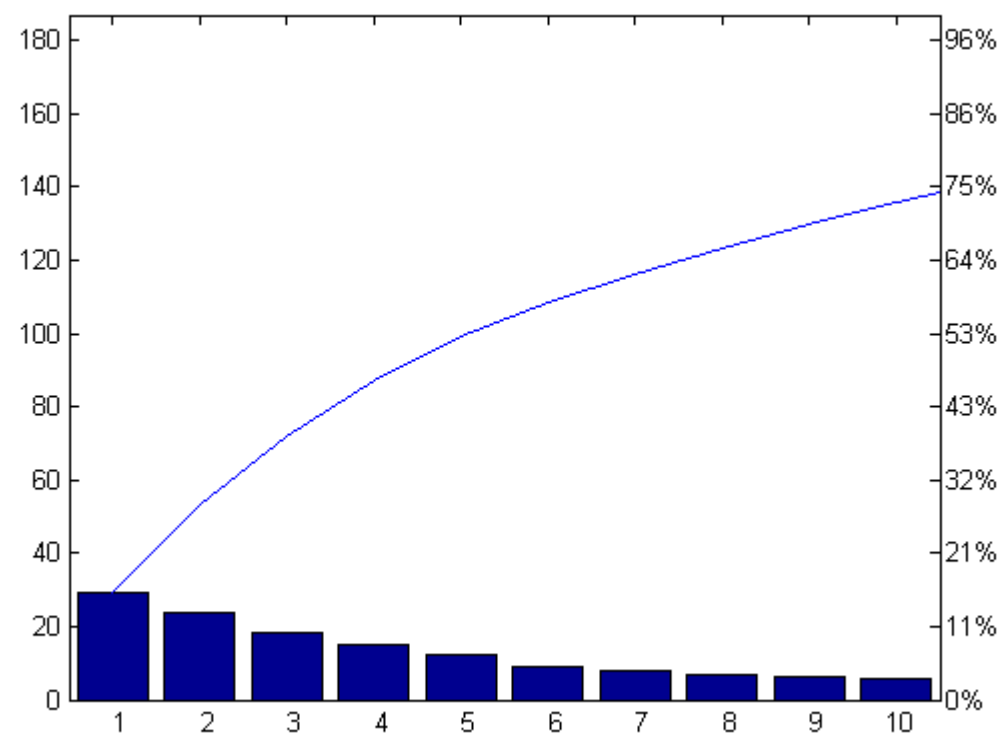
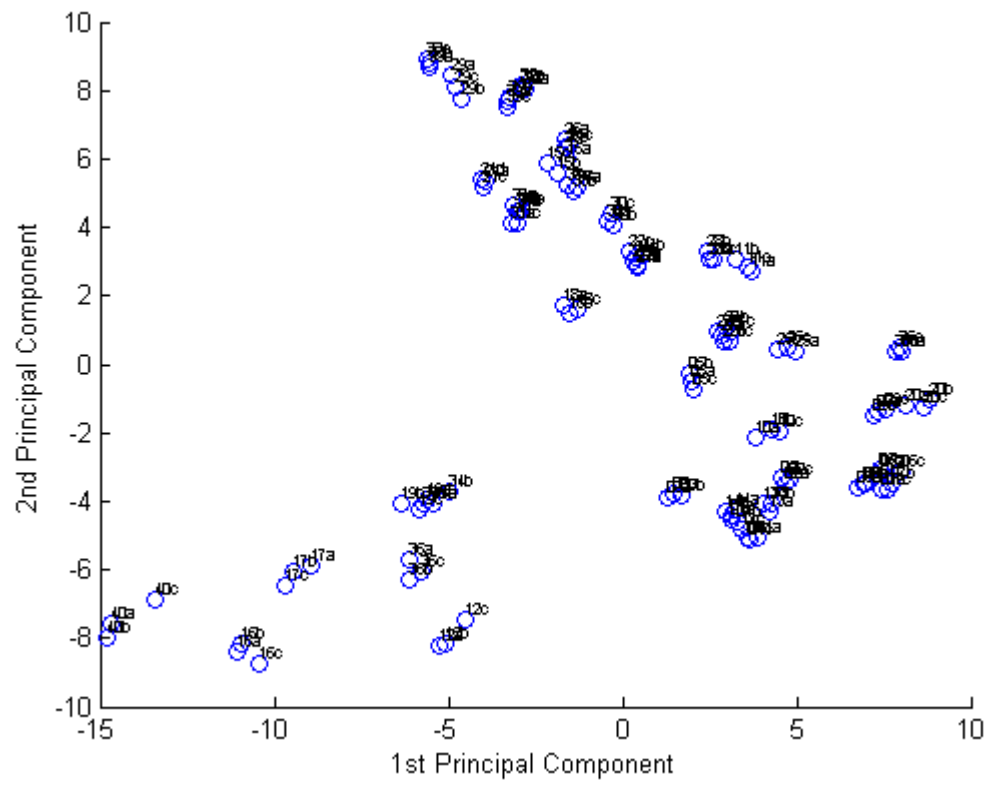

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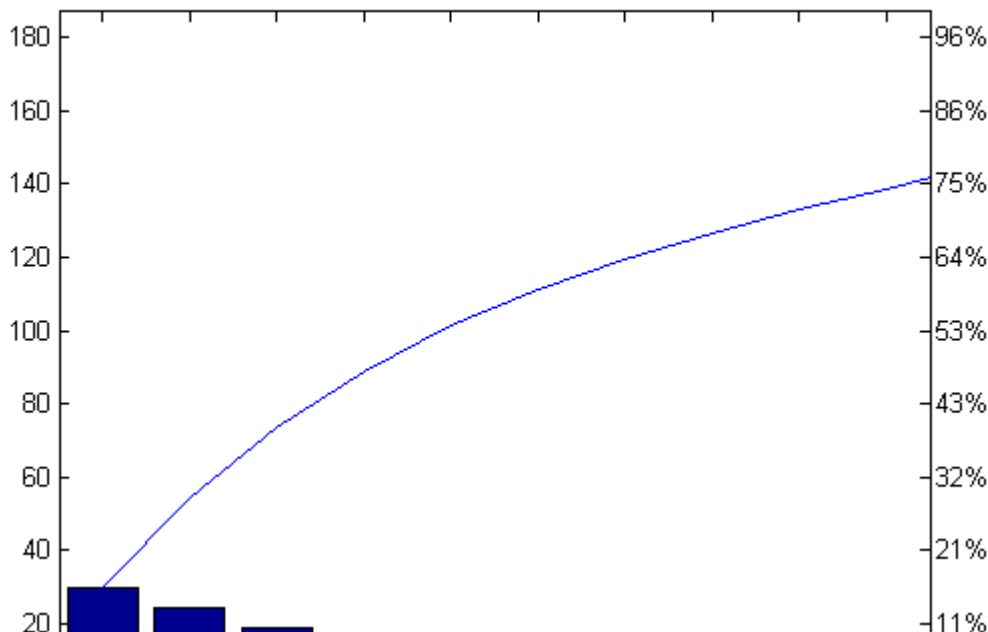
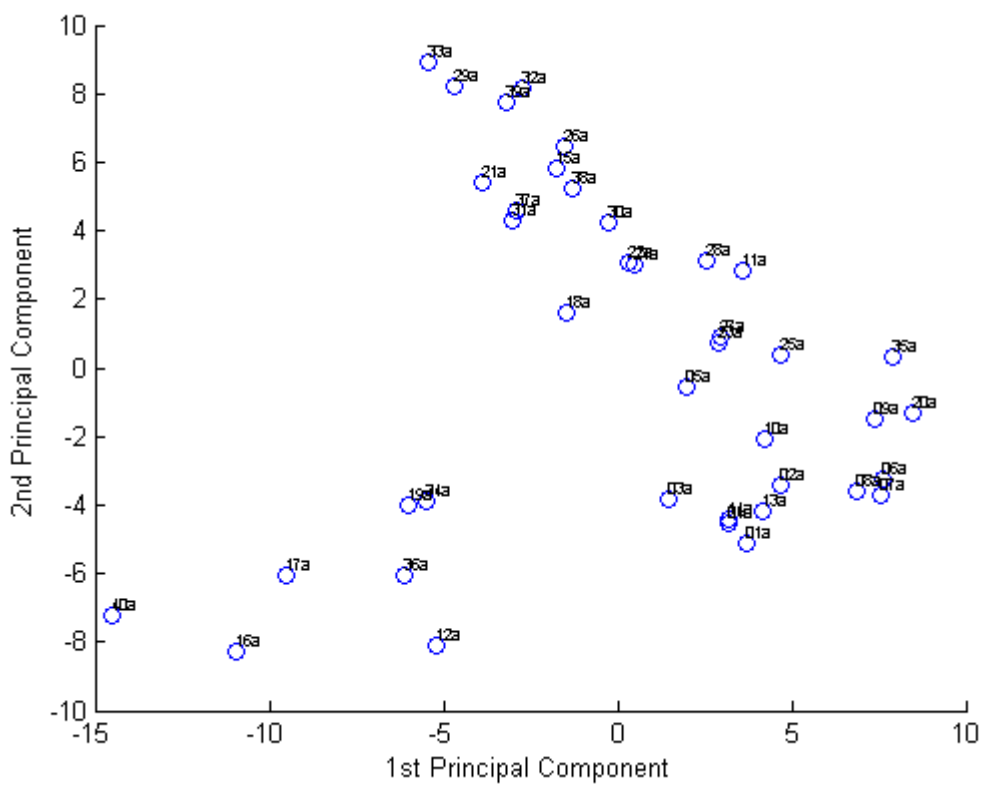
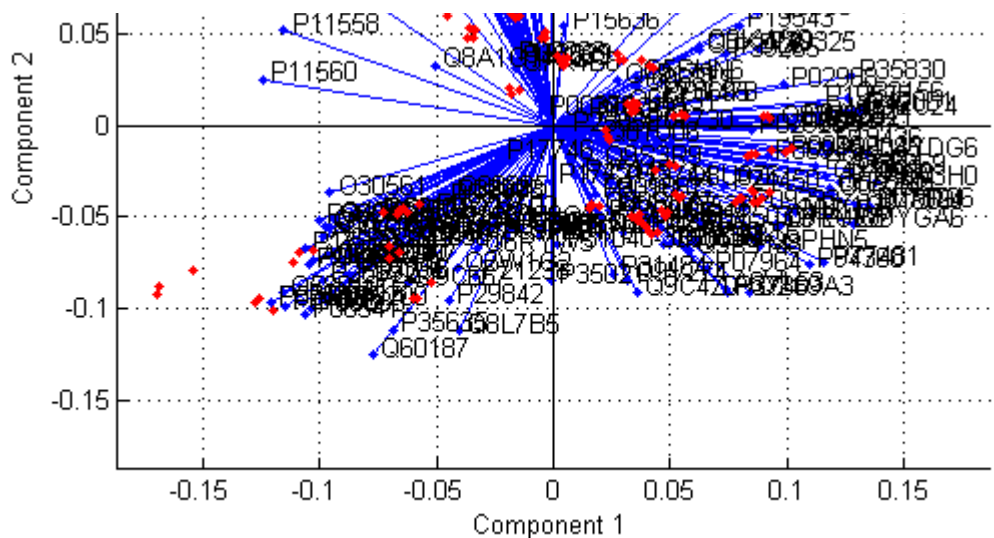
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READ: Gent_MP_UniRef50_allSpecies_Gent09b
READ: Gent_MP_UniRef50_allSpecies_Gent09c
READ: Gent_MP_UniRef50_allSpecies_Gent10a
READ: Gent_MP_UniRef50_allSpecies_Gent10b
READ: Gent_MP_UniRef50_allSpecies_Gent10c
READ: Gent_MP_UniRef50_allSpecies_Gent11a
READ: Gent_MP_UniRef50_allSpecies_Gent11b
READ: Gent_MP_UniRef50_allSpecies_Gent11c
READ: Gent_MP_UniRef50_allSpecies_Gent12a
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READ: Gent_MP_UniRef50_allSpecies_Gent13a
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READ: Gent_MP_UniRef50_allSpecies_Gent13c
READ: Gent_MP_UniRef50_allSpecies_Gent14a
READ: Gent_MP_UniRef50_allSpecies_Gent14b
READ: Gent_MP_UniRef50_allSpecies_Gent14c
READ: Gent_MP_UniRef50_allSpecies_Gent15a
READ: Gent_MP_UniRef50_allSpecies_Gent15b
READ: Gent_MP_UniRef50_allSpecies_Gent15c
READ: Gent_MP_UniRef50_allSpecies_Gent16a
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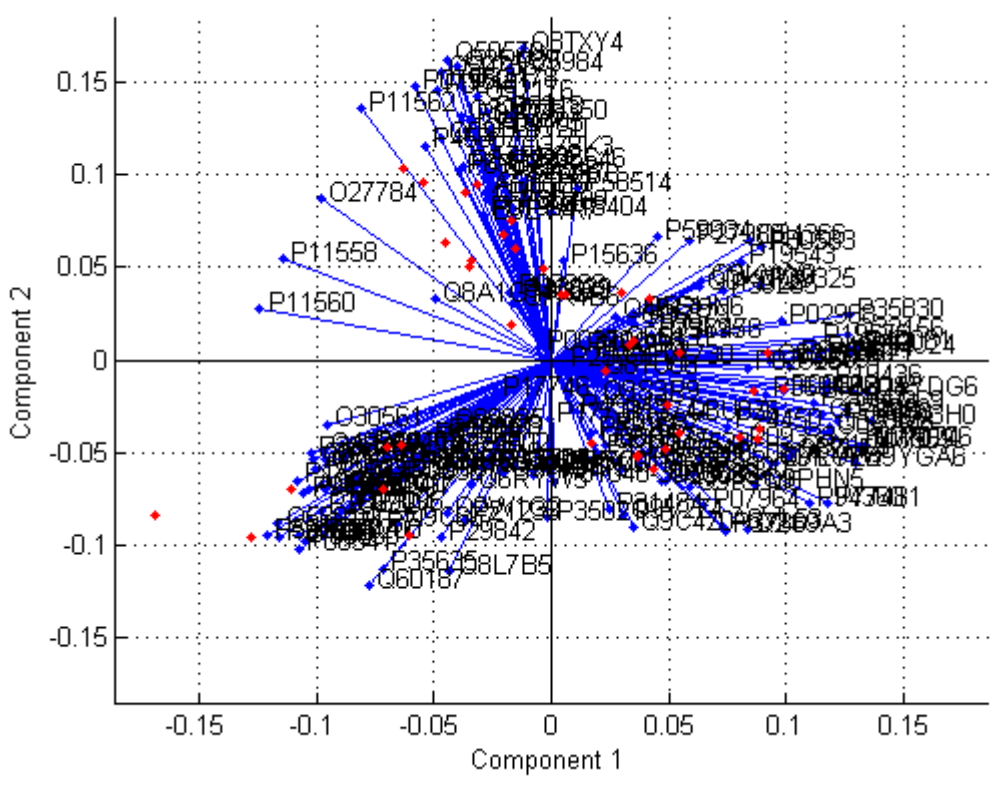
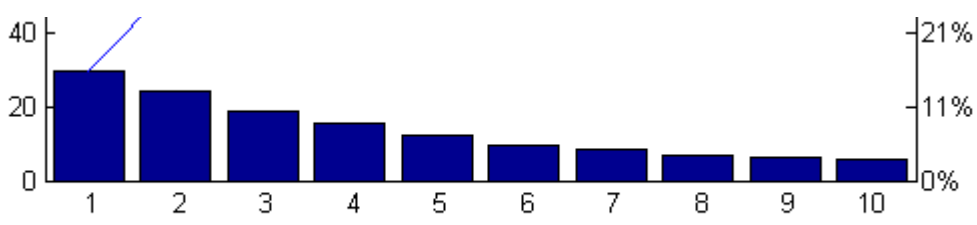
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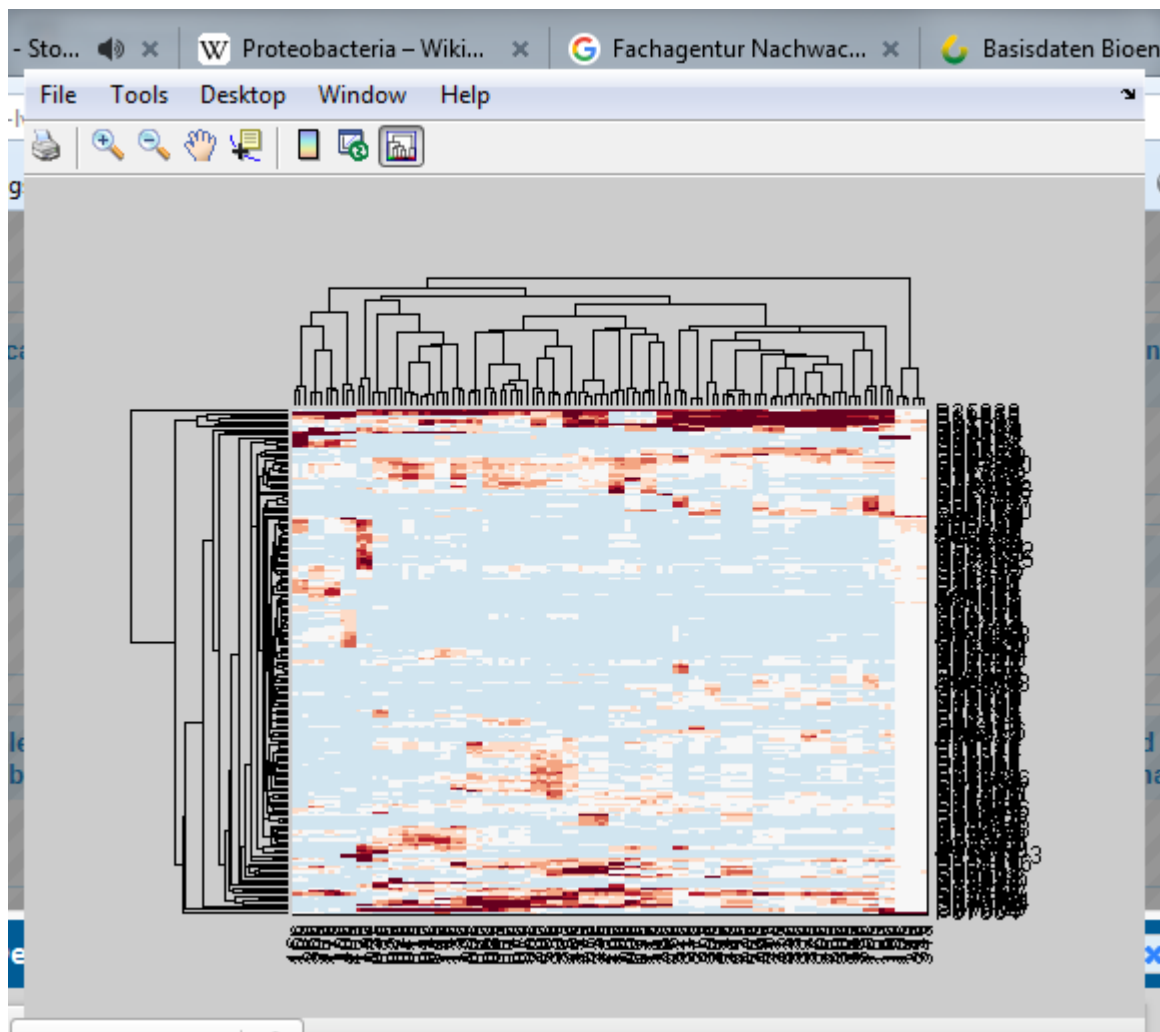
MetaProtein files successfully read:

Matrix was normalized and filtered by threshold 0.01 successfully
CrossCorrelation with Spearman matrix successfully calculated









Perform mixed correlations necessary that both matrixes has the same number of entries

Metadata

```
[meta_taxo_correlationMatrix ] = CalculateCorrelation_V2(meta_matrix, tax_average_matrix_filt
[meta_onto_correlationMatrix ] = CalculateCorrelation_V2(meta_matrix, onto_average_matrix_fil
[meta_mp_correlationMatrix ] = CalculateCorrelation_V2(meta_matrix, mp_average_matrix_filtere
% Taxodata
[taxo_meta_correlationMatrix ] = CalculateCorrelation_V2(tax_average_matrix_filtered, meta_ma
[taxo_onto_correlationMatrix ] = CalculateCorrelation_V2(tax_average_matrix_filtered, onto_av
[taxo_mp_correlationMatrix ] = CalculateCorrelation_V2(tax_average_matrix_filtered, mp_averag
% Ontodata
[onto_meta_correlationMatrix] = CalculateCorrelation_V2(onto_average_matrix_filtered,meta_mat
[onto_taxo_correlationMatrix ] = CalculateCorrelation_V2(onto_average_matrix_filtered,tax_ave
[onto_mp_correlationMatrix ] = CalculateCorrelation_V2(onto_average_matrix_filtered, mp_avera
% MPdata
[mp_meta_correlationMatrix ] = CalculateCorrelation_V2(mp_average_matrix_filtered,meta_matrix
[mp_taxo_correlationMatrix ] = CalculateCorrelation_V2(mp_average_matrix_filtered,tax_average
[mp_onto_correlationMatrix ] = CalculateCorrelation_V2(mp_average_matrix_filtered, onto_avera
```

```
CrossCorrelation with Spearman matrix successfully calculated
CrossCorrelation with Spearman matrix successfully calculated
CrossCorrelation with Spearman matrix successfully calculated
CrossCorrelation with Spearman matrix successfully calculated
CrossCorrelation with Spearman matrix successfully calculated
CrossCorrelation with Spearman matrix successfully calculated
CrossCorrelation with Spearman matrix successfully calculated
CrossCorrelation with Spearman matrix successfully calculated
```

```
CrossCorrelation with Spearman matrix successfully calculated  
CrossCorrelation with Spearman matrix successfully calculated  
CrossCorrelation with Spearman matrix successfully calculated  
CrossCorrelation with Spearman matrix successfully calculated  
CrossCorrelation with Spearman matrix successfully calculated  
CrossCorrelation with Spearman matrix successfully calculated  
CrossCorrelation with Spearman matrix successfully calculated
```

FINISH

```
disp('Finish')
```

Finish

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