PEC1

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En este trabajo se realizará un análsis exploratorio de un estudio metabolómico, escogido desde la base de datos **Metabolomics Workbench**. Por otro lado, usaremos la librerías **metabolomicsWorkbenchR** para extraer los datos directamente desde la web y **SummarizedExperiment** para manejar los datos de manera estructurada. ambas librerías se encuentran en el repositorio **Bioconductor**. Para utilizar estas librerías, primero asegurarse de tener instalado Bioconductor y luego instalar metabolomicsWorkbenchR y SummarizedExperiment como indica en sus respectivos links.

Importación de librería

```
library(metabolomicsWorkbenchR)
library(SummarizedExperiment)
```

Estudios Disponibles

```
estudios = do_query(
    context = 'study',
    input_item = 'study_title',
    input_value = 'Bacterial',
    output_item = 'summary'
)
```

Summary de estudio seleccionado

```
summary <- do_query(
    context = "study",
    input_item = "study_id",
    input_value = "ST003521",
    output_item = "summary"
)
```

Carga de Datos en clase SummarizedExperiment

```
SE = do_query(
    context = 'study',
    input_item = 'study_id',
    input_value = 'ST003521',
    output_item = 'SummarizedExperiment'
)
```

```
print(head(rowData(SE$AN005782)))
```

```
## DataFrame with 6 rows and 3 columns
##                 metabolite_name metabolite_id            refmet_name
##                     <character>   <character>            <character>
## ME917515 10,11-dihydro-20-tri..      ME917515
## ME917423 1-(14-methyl-pentade..      ME917423
## ME917123 1,2-dihexadecanoyl-s..      ME917123
## ME917224 1,3,5-trimethoxybenz..      ME917224 1,3,5-Trimethoxybenz..
## ME917120      1-4-beta-D-Glucan      ME917120      1,4-beta-D-Glucan
## ME917031 1,6-anhydro-N-acetyl..      ME917031
```

```
#print(head(rowData(SE$AN005783)))
```

```
print(head(colData(SE$AN005782)))
```

```
## DataFrame with 6 rows and 7 columns
##          local_sample_id    study_id  sample_source mb_sample_id    raw_data
##              <character> <character>    <character>  <character> <character>
## Blank_1          Blank_1    ST003521        _BLANK_     SA386750
## Blank_2          Blank_2    ST003521        _BLANK_     SA386751
## Blank_3          Blank_3    ST003521        _BLANK_     SA386752
## Blank_4          Blank_4    ST003521        _BLANK_     SA386753
## Blank_5          Blank_5    ST003521        _BLANK_     SA386754
## COM_1h_1        COM_1h_1    ST003521 Combination_1h     SA386726
##              Sample_source raw_file_name
##                  <factor>      <factor>
## Blank_1  Extraction blank       Blank_1
## Blank_2  Extraction blank       Blank_2
## Blank_3  Extraction blank       Blank_3
## Blank_4  Extraction blank       Blank_4
## Blank_5  Extraction blank       Blank_5
## COM_1h_1 Combination_1h         COM_1h_1
```

```
#print(head(colData(SE$AN005783)))
```

```
print(head(metadata(SE$AN005782)))
```

```
## $data_source
## [1] "Metabolomics Workbench"
##
## $study_id
## [1] "ST003521"
```

```
##
## $analysis_id
## [1] "AN005782"
##
## $analysis_summary
## [1] "HILIC POSITIVE ION MODE"
##
## $units
## [1] "peak height"
##
## $name
## [1] "ST003521:AN005782"
```

```
#print(head(metadata(SE$AN005783)))
```

```
print(head(assay(SE$AN005782)))
```

```
##    Blank_1 Blank_2 Blank_3 Blank_4 Blank_5 COM_1h_1 COM_1h_2 COM_1h_3 COM_1h_4
##      <num>   <num>   <num>   <num>   <num>    <num>    <num>    <num>    <num>
## 1:      NA      NA      NA      NA      NA   280668   179652   152334   186482
## 2:      NA      NA      NA      NA      NA    49312    52133    54610    16889
## 3:   12395      NA      NA      NA      NA    22367  1054362   127405  7622910
## 4:      NA      NA      NA      NA      NA    12447       NA     9947       NA
## 5:      NA      NA      NA      NA      NA    92754   151013   108064   177670
## 6:   19383      NA      NA   15656      NA   159694   222957   246475   178822
##    COM_3h_1 COM_3h_2 COM_3h_3 COM_3h_4 COM_6h_1 COM_6h_2 COM_6h_3 COM_6h_4
##       <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1:   452100   733604   420211   450253   431965   388727   601752   388851
## 2:    86925    73106    52103    76944    65142    59515    76767    68061
## 3:  1115624   874283  6799985   870091  1522665  4207413   604828  5465581
## 4:    15240    48843    33415    24876    45447    12455    28990    11414
## 5:   138774   171814   189911   175622   119701   130112   136338   139970
## 6:   208951   237917   190438   249728   292673   336180   226382   264382
##    Control_1h_1 Control_1h_2 Control_1h_3 Control_1h_4 Control_3h_1
##           <num>        <num>        <num>        <num>        <num>
## 1:      1818857      1375962      1509317      1681759       884417
## 2:       106742       102989       103047       120336       118662
## 3:      3847236      4486209      1516420      1830488       106654
## 4:        84947       128149        60962        65129       124665
## 5:       442106       409274       481459       361730       122187
## 6:       443963       331631       457979       505645       272411
##    Control_3h_2 Control_3h_3 Control_3h_4 Control_6h_1 Control_6h_2
##           <num>        <num>        <num>        <num>        <num>
## 1:       794581      1994645      1348747       467774       663895
## 2:       108991        81850       113313       101862       104434
## 3:       965914      6384843       506936       367294      2919519
## 4:       237731        78899       108125       246021        89555
## 5:       202180       354376       266421        99922       201860
## 6:       266485       301057       315926       189732       295567
##    Control_6h_3 Control_6h_4 PMB_1h_1  PMB_1h_2   PMB_1h_3   PMB_1h_4  PMB_3h_1
##           <num>        <num>    <num>     <num>      <num>      <num>     <num>
## 1:       784321       835575   269053 585805.12  605523.81  757481.38 193776.84
## 2:       131257        97158    64934  71493.54   72008.92   47840.11  78057.03
```

```
## 3:       600041       707990   629381 249339.69 2021466.25 8257482.50 737428.44
## 4:       172785        98790    10144  24189.11   14465.55         NA  15076.38
## 5:       181206       188752   112056 103789.20  187231.88  189065.73 129670.80
## 6:       247358       144490   251053 216165.17  339886.66  317651.50 513024.03
##     PMB_3h_2  PMB_3h_3   PMB_3h_4   PMB_6h_1  PMB_6h_2   PMB_6h_3  PMB_6h_4
##        <num>     <num>      <num>      <num>     <num>      <num>     <num>
## 1: 244367.77 273454.25  450595.75  257433.80 234823.47  366864.47 156483.89
## 2:  88198.67  88070.41   68595.87   27290.17  84942.77   73122.06  89298.75
## 3: 233692.16 413207.22 2721615.25 9374632.00 459783.38 1253944.25 175183.91
## 4:  12003.70  19639.07   12696.07   13465.14  49697.35   34237.33  17987.28
## 5: 132373.16 186734.38  493180.56  120960.38  75497.72  188186.59  51642.46
## 6: 620721.75 754682.38 1054005.12  324754.56 636336.56  652709.19 553809.44
##         QC_1      QC_2      QC_3      QC_4       QC_5    TX_1h_1   TX_1h_2
##        <num>     <num>     <num>     <num>      <num>      <num>     <num>
## 1: 1853824.2 1553839.1 1535762.4 1698413.5  881474.88 1368279.12 798333.44
## 2:  126771.1  182426.8  207763.0  217815.1   91794.55  121270.77  89541.43
## 3: 1981206.6 2417474.8 2593358.5 2272343.8 1803045.88  425224.91 693338.69
## 4:  138008.5  211598.0  159640.0  174708.3  141130.84   73381.91  57658.30
## 5:  289663.1  602814.6  568196.2  510402.7  256229.20  282749.97 291757.94
## 6: 2716046.0  490059.3  527350.2  537212.2  493097.28  617145.06 476714.69
##       TX_1h_3    TX_1h_4  TX_3h_1   TX_3h_2  TX_3h_3    TX_3h_4   TX_6h_1
##         <num>      <num>    <num>     <num>    <num>      <num>     <num>
## 1: 1856543.00 1409286.25 545794.0 516368.72 887164.4  909613.81 777604.31
## 2:   88246.15   97507.39 100288.5  92955.97 101954.7   98742.24 110264.81
## 3: 2045336.88  450899.97 144449.9 704337.00 679523.2 1846743.75 432232.50
## 4:   67583.39   77058.89 212783.2 124644.37 135956.6   74438.63  85776.06
## 5:  492493.31  328415.31 156992.0 229934.44 292763.8  323432.88 122845.92
## 6:  612405.00  506788.19 352351.2 403477.69 439974.3  459863.44 421238.94
##      TX_6h_2   TX_6h_3  TX_6h_4
##        <num>     <num>    <num>
## 1: 466885.12 451567.16 788775.3
## 2:  81395.59  98310.16  77048.6
## 3: 609650.62 292579.12 426231.8
## 4:  40105.14  60916.61 118543.6
## 5: 132327.39 128582.52 158017.6
## 6: 534918.94 362823.56 420443.3
```

```
#print(head(assay(SE$AN005783)))
```