

Untitled1

Source on Save Run Source

1

This is the first time you open the Rstudio
The interface may be a little different from yours

1:1 (Top Level) R Script

Files Plots Packages Help Viewer

New Folder Delete Rename More

Home

Console Terminal

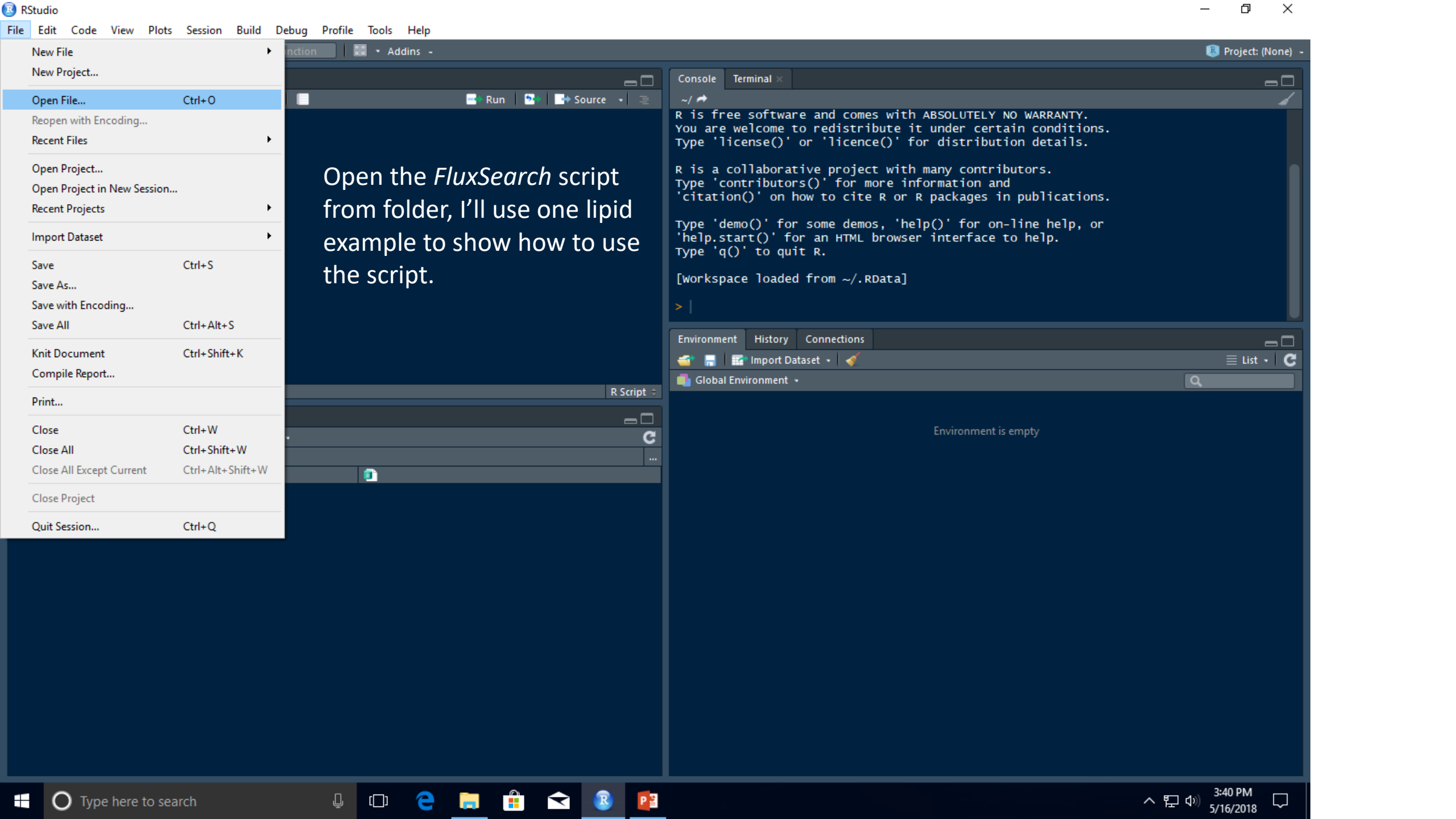
```
~/  
R is free software and comes with ABSOLUTELY NO WARRANTY.  
You are welcome to redistribute it under certain conditions.  
Type 'license()' or 'licence()' for distribution details.  
  
R is a collaborative project with many contributors.  
Type 'contributors()' for more information and  
'citation()' on how to cite R or R packages in publications.  
  
Type 'demo()' for some demos, 'help()' for on-line help, or  
'help.start()' for an HTML browser interface to help.  
Type 'q()' to quit R.  
  
[workspace loaded from ~/.RData]  
  
> |
```

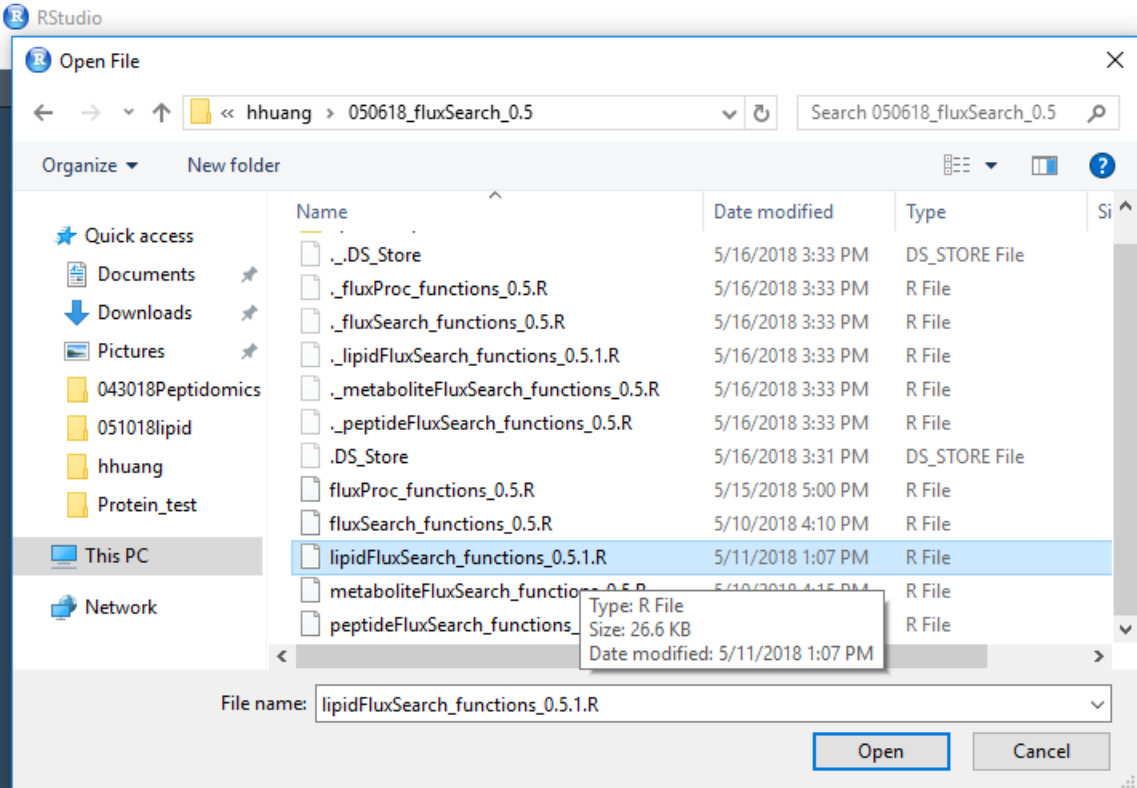
Environment History Connections

Import Dataset

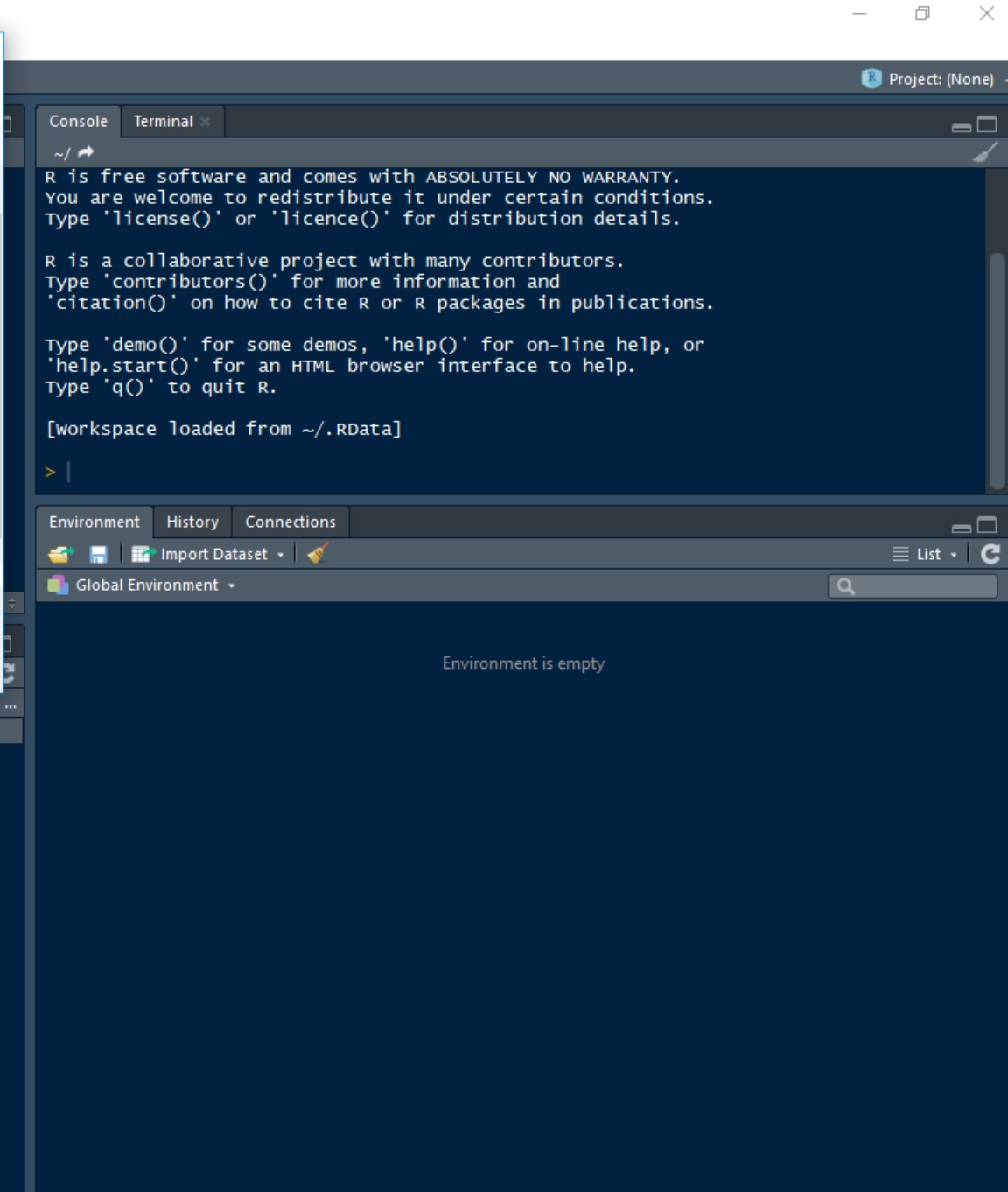
Global Environment

Environment is empty





Select the *lipidFluxSearch_functions* as I am using the lipid samples this time



FileEditCodeViewPlotsSessionBuildDebugProfileToolsHelp

Go to file/function

Addins

Project: (None)

lipidFluxSearch_functions_0.5.1.R

```
1 require(fuzzyjoin)
2 require(data.table)
3 require(dplyr)
4
5
6
7
8
9 # =====
10 # Build the isotopomer reference files (40 carbon)
11 # Positive mode
12 refLibPos_ls <- function(refInput) {
13   refPeaklist <- fread(refInput)
14   # extract the positive peaks for reference positive files
15   refPeaklist_pos <- subset(refPeaklist, refPeaklist$Pol == "p")
16   # re-organize the refPeaklist_pos
17   mz2 <- refPeaklist_pos$ObsMz
18   rt2 <- refPeaklist_pos$Rt
19   Lipid <- refPeaklist_pos$LipidIon
20   # ...
21 }
```

1:1 (Top Level) R Script

ConsoleTerminal

```
~/
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Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

[workspace loaded from ~/.RData]

> |
```

EnvironmentHistoryConnections

Import Dataset

Global Environment

Environment is empty

FilesPlotsPackagesHelpViewer

New FolderDeleteRenameMore

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This is how the script looks like
lipidFluxSearch_functions

RStudio

File Edit Code View Plots Session Build Debug Profile Tools Help

Go to file/function Addins

Untitled1* x lipidFluxSearch_functions_0.5.1.R x

Source on Save Run Source

```
1 install.packages(c("fuzzyjoin", "data.table", "dplyr"))
```

1:56 (Top Level) R Script

Files Plots Packages Help Viewer

New Folder Delete Rename More

Home

BUT!!!! Before you use the script, you need to install some dependent R packages for *FluxSearch*. Simply type this line as above.

Project: (None)

Console Terminal x

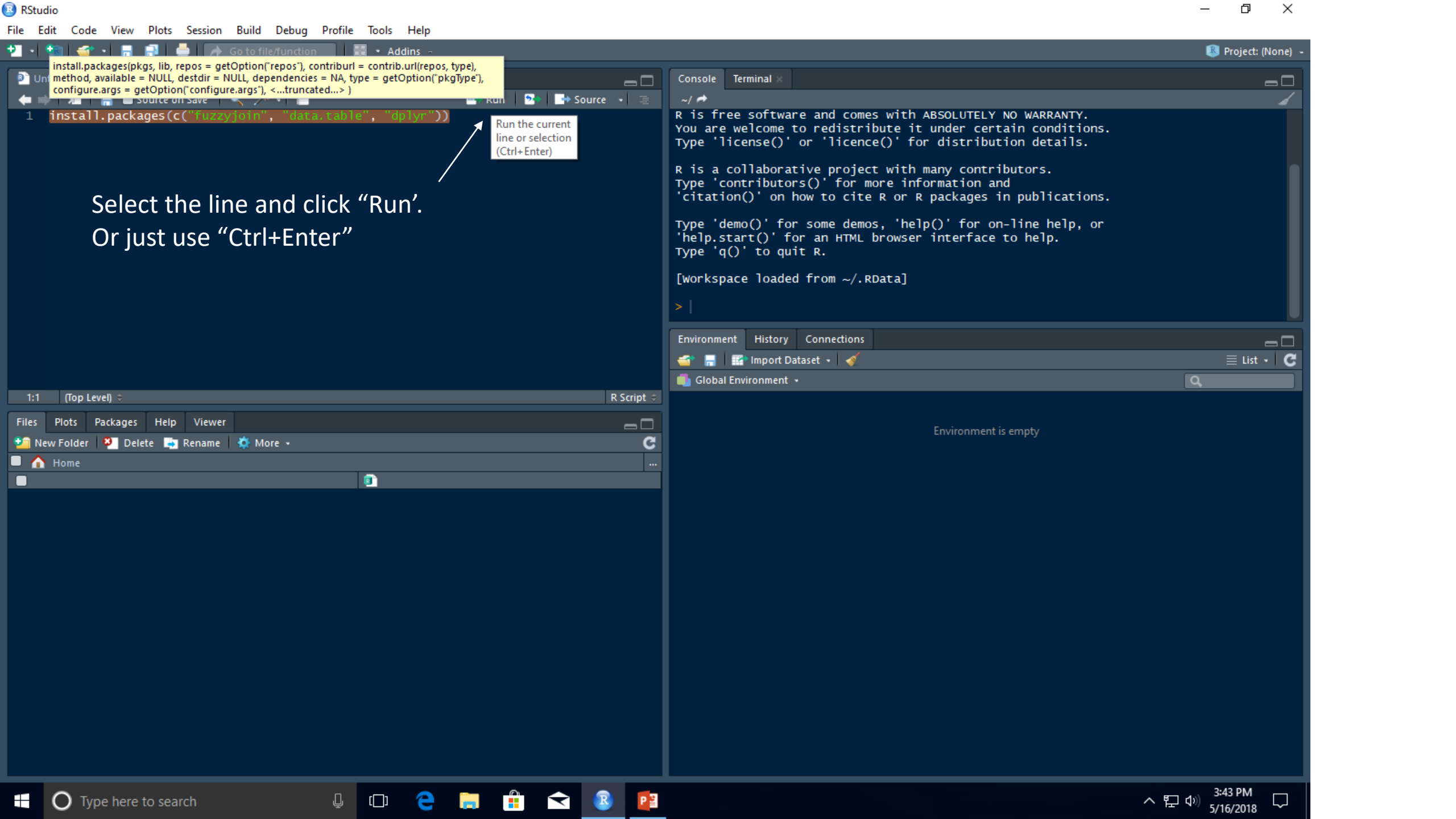
```
~/  
R is free software and comes with ABSOLUTELY NO WARRANTY.  
You are welcome to redistribute it under certain conditions.  
Type 'license()' or 'licence()' for distribution details.  
  
R is a collaborative project with many contributors.  
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Type 'demo()' for some demos, 'help()' for on-line help, or  
'help.start()' for an HTML browser interface to help.  
Type 'q()' to quit R.  
  
[workspace loaded from ~/.RData]  
  
> |
```

Environment History Connections

Import Dataset

Global Environment

Environment is empty



RStudio

File Edit Code View Plots Session Build Debug Profile Tools Help

Go to file/function Addins

Project: (None)

Untitled1* x lipidFluxSearch_functions_0.5.1.R x

Source on Save Run Source

```
1 require(fuzzyjoin)
2 require(data.table)
3 require(dplyr)
4
5
6
7
8
9 # =====
10 # Build the isotopomer reference files (40 carbon)
11 # Positive mode
12 refLibPos_ls <- function(refInput) {
13   refPeaklist <- fread(refInput)
14   # extract the positive peaks for reference positive files
15   refPeaklist_pos <- subset(refPeaklist, refPeaklist$Pol == "p")
16   # re-organize the refPeaklist_pos
17   mz2 <- refPeaklist_pos$ObsMz
18   rt2 <- refPeaklist_pos$Rt
19   Lipid <- refPeaklist_pos$LipidIon
20   Extended <- refPeaklist_pos$Extended
21 }
```

484:1 # (Untitled) R Script

Files Plots Packages Help Viewer

New Folder Delete Rename More

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Environment History Connections

Import Dataset

Global Environment

Environment is empty

Console Terminal

~/

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Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

[workspace loaded from ~/.RData]

> |

If this is not your first time to use *FluxSearch*, you can skip the former step, and go to the script directly.

FileEditCodeViewPlotsSessionBuildDebugProfileToolsHelp

Go to file/functionAddins

Project: (None)

Untitled1*lipidFluxSearch_functions_0.5.1.R

Source on SaveRunSource

```
1 require(fuzzyjoin)
2 require(data.table)
3 require(dplyr)
4
5
6
7
8
9 #####
10 # Build the isotopomer reference files (40 carbon)
11 # Positive mode
12 refLibPos_ls <- function(refInput) {
13   refPeaklist <- fread(refInput)
14   # extract the positive peaks for reference positive files
15   refPeaklist_pos <- subset(refPeaklist, refPeaklist$Pol == "p")
16   # re-organize the refPeaklist_pos
17   mz2 <- refPeaklist_pos$ObsMZ
18   rt2 <- refPeaklist_pos$Rt
19   Lipid <- refPeaklist_pos$LipidIon
20   # ...
21 }
```

ConsoleTerminal

~/

```
between, first, last

The following objects are masked from 'package:stats':

  filter, lag

The following objects are masked from 'package:base':

  intersect, setdiff, setequal, union

Warning messages:
1: package 'fuzzyjoin' was built under R version 3.4.4
2: package 'data.table' was built under R version 3.4.4
> |
```

EnvironmentHistoryConnections

Import Dataset

Global Environment

Functions

Flux_result	function (input_negative, input_positive, referInput, sco...
mmf	function (x, y)
msMatch	function (mzFile, refFile)
ref_13C_neg	function (refInput, refOutput)
ref_13C_pos	function (refInput, refOutput)
refLibNeg_ls	function (refInput)
refLibPos_ls	function (refInput)
resultwrap_neg	function (inputFile_neg, refInput)
resultwrap_pos	function (inputFile_pos, refInput)
Sgrade	function (inputResult)

FilesPlotsPackagesHelpViewer

New FolderDeleteRenameMore

Home

Type here to search

3:44 PM 5/16/2018


```
=====
wrap all positive and negative files together

Flux_result <- function(input_negative, input_positive, referInput, score = 0.8) {
  flux_neg <- resultwrap_neg(input_negative, referInput)
  flux_pos <- resultwrap_pos(input_positive, referInput)
  output_all <- rbind(flux_neg, flux_pos)
  output_all <- Sgrade(output_all)
  # select feature with good grades
  output_all <- subset(output_all, output_all$Score >= score)

  return(output_all)
}

Grading function
grade <- function(inputResult) {
  inputResult$grades <- Flux_result(inputResult$neg, inputResult$pos, inputResult$ref, 0.8)
}

Flux_result(input_negative, input_positive, referInput, score)
```

The only function you need to use in this script is the one highlighted – “Flux_result” which has four attributes:

1. input_negative,
2. Input_positive,
3. referInput,
4. score

```
~/
between, first, last

The following objects are masked from 'package:stats':
  filter, lag

The following objects are masked from 'package:base':
  intersect, setdiff, setequal, union

warning messages:
1: package 'fuzzyjoin' was built under R version 3.4.4
2: package 'data.table' was built under R version 3.4.4
> |
```

Environment	History	Connections
Import Dataset		
Global Environment		
Functions		
Flux_result	function (input_negative, input_positive, referInput,	
mmf	function (x, y)	
msMatch	function (mzFile, refFile)	
ref_13C_neg	function (refInput, refOutput)	
ref_13C_pos	function (refInput, refOutput)	
refLibNeg_ls	function (refInput)	
refLibPos_ls	function (refInput)	
resultwrap_neg	function (inputFile_neg, refInput)	
resultwrap_pos	function (inputFile_pos, refInput)	
Sgrade	function (inputResult)	

RStudio

File Edit Code View Plots Session Build Debug Profile Tools Help

Go to file/function Addins

Untitled1* x lipidFluxSearch_functions_0.5.1.R x

Source on Save Run Source

```
1 install.packages(c("fuzzyjoin", "data.table", "dplyr"))
2
3 Pah11_lipid <- |
```

To use this function, you may want to create a object to save the result on RAM, otherwise you may not find your result if something unexpected happens. In this case, I'll just create a object named "Pah11_lipid" and add a "<-" sign after it.

3:16 (Top Level) R Script

Files Plots Packages Help Viewer

New Folder Delete Rename More

Home

Project: (None)

Console Terminal x

```
~/
between, first, last

The following objects are masked from 'package:stats':
  filter, lag

The following objects are masked from 'package:base':
  intersect, setdiff, setequal, union

Warning messages:
1: package 'fuzzyjoin' was built under R version 3.4.4
2: package 'data.table' was built under R version 3.4.4
> |
```

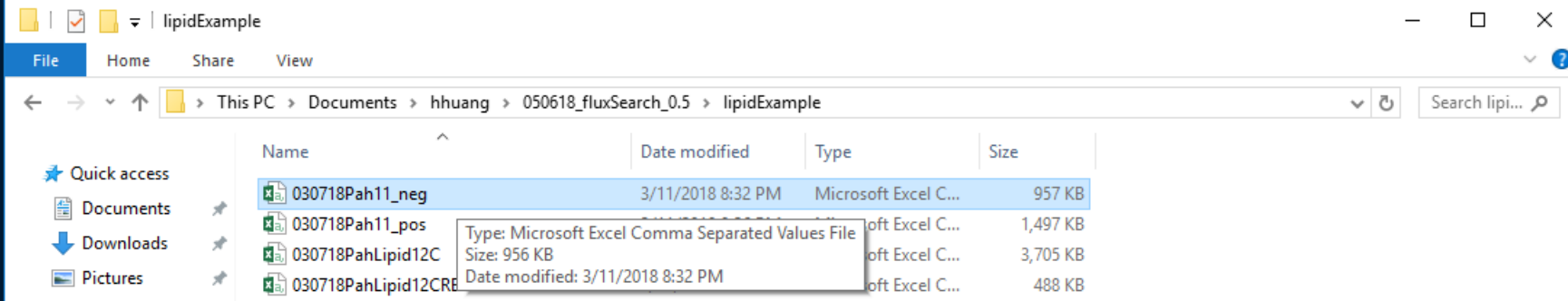
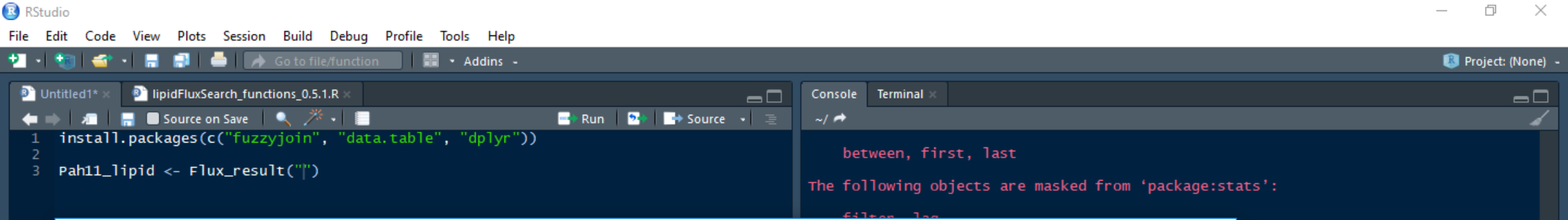
Environment History Connections

Import Dataset

Global Environment

Functions

Flux_result	function (input_negative, input_positive, referInput, sco...
mmf	function (x, y)
msMatch	function (mzFile, refFile)
ref_13C_neg	function (refInput, refOutput)
ref_13C_pos	function (refInput, refOutput)
refLibNeg_ls	function (refInput)
refLibPos_ls	function (refInput)
resultwrap_neg	function (inputFile_neg, refInput)
resultwrap_pos	function (inputFile_pos, refInput)
Sgrade	function (inputResult)



Now I'm add the function after my object "Pah11_lipid", just type "Flux_result(...)" after the "<-"

The first attribute is sample negative peaklist, so you need to enter the path of the negative peaklist of your sample.

```
1 install.packages(c("fuzzyjoin", "data.table", "dplyr"))
2
3 Pah11_lipid <- Flux_result("c:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_neg.csv")
```

the path of the negative peaklist of
your sample.

Console

```
~/
ge:stats':
  filter, lag

The following objects are masked from 'package:base':
  intersect, setdiff, setequal, union

Warning messages:
1: package 'fuzzyjoin' was built under R version 3.4.4
2: package 'data.table' was built under R version 3.4.4
> |
```

Environment History Connections

Import Dataset

Global Environment

Functions

Flux_result	function (input_negative, i...
mmf	function (x, y)
msMatch	function (mzFile, refFile)
ref_13C_neg	function (refInput, refoutp...
ref_13C_pos	function (refInput, refoutp...
refLibNeg_...	function (refInput)
refLibPos_...	function (refInput)
resultwrap...	function (inputFile_neg, re...
resultwrap...	function (inputFile_pos, re...
Sgrade	function (inputResult)

```
1 install.packages(c("fuzzyjoin", "data.table", "dplyr"))
2
3 pah11_lipid <- Flux_result("c:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipid
4 )
```

Console Terminal

~/

```
between, first, last
The following objects are masked from 'package:stats':
  filter, lag
```

lipidExample

File Home Share View

This PC > Documents > hhuang > 050618_fluxSearch_0.5 > lipidExample

Name	Date modified	Type	Size
030718Pah11_neg	3/11/2018 8:32 PM	Microsoft Excel C...	957 KB
030718Pah11_pos	3/11/2018 8:26 PM	Microsoft Excel C...	1,497 KB
030718PahLipid12C	3/11/2018 8:26 PM	Microsoft Excel C...	3,705 KB
030718PahLipid12CREP	3/11/2018 8:26 PM	Microsoft Excel C...	488 KB

Type: Microsoft Excel Comma Separated Values File
Size: 1.46 MB
Date modified: 3/11/2018 8:26 PM

The second attribute is sample positive peaklist, so you need to enter the path of the positive peaklist of your sample.

```
ge:base':
version 3.4.4
version 3.4.4

ve, input_positive, referInput,...
file)
foutput)
foutput)

g, refInput)
s, refInput)
```

```
1 install.packages(c("fuzzyjoin", "data.table", "dplyr"))
2
3 Pah11_lipid <- Flux_result("C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_neg.csv",
4                           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_pos.csv",
5                           )
```

the path of the positive peaklist of
your sample.

Console Terminal

```
~/
```

filter, lag

The following objects are masked from 'package:base':

intersect, setdiff, setequal, union

Warning messages:

```
1: package 'fuzzyjoin' was built under R version 3.4.4
2: package 'data.table' was built under R version 3.4.4
> |
```

Environment History Connections

Import Dataset List

Global Environment

Functions

Flux_re...	function (input_neg...	
mmf	function (x, y)	
msMatch	function (mzFile, r...	
ref_13C...	function (refInput,...	
ref_13C...	function (refInput,...	
refLibN...	function (refInput)	
refLibP...	function (refInput)	
resultw...	function (inputFile...	
resultw...	function (inputFile...	
Sgrade	function (inputResu...	

5:28 (Top Level)

R Script

Files Plots Packages Help Viewer

File Home Share View

Name	Date modified	Type	Size
------	---------------	------	------

Documents	030718Pah11_neg	3/11/2018 8:32 PM	Microsoft Excel C...	957 KB
-----------	-----------------	-------------------	----------------------	--------

Pictures	030718PahLipid12C	3/11/2018 6:29 PM	Microsoft Excel C...	3,705 KB
	030718P-H11-M12GRFF	3/16/2018 2:22 PM	Microsoft Excel C...	400 KB

Type: Microsoft Excel Comma Separated Values File

nhuang

The third attribute is 136 reference

list, so you need to enter the path of

the 12C reference.

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Files

Windows taskbar with search bar and application icons (Edge, File Explorer, Mail, etc.)

~ / ↩

filter, lag

```
from package:base:
```

union

```
1: package 'fuzzyjoin' was built  
under R version 3.4.4
```

```
under R version 3.4.4
>
```

Environment History Connections

Global Environment

```
Flux_re... function (input_neg...  
mmf      function (x, y)
```

```
ref_13C... function (refInput, ...)
```

```
refLibN... function (refInput)
refLibN... function (refInput)
```

```
resultw... function (inputFile...
```

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3:49 PM

```
1 install.packages(c("fuzzyjoin", "data.table", "dplyr"))
2
3 Pah11_lipid <- Flux_result("C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_neg.csv",
4                           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_pos.csv",
5                           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718PahLipid12CREf.csv")
```

the path of the 12C reference

Console Terminal

```
~/
```

filter, lag

The following objects are masked from 'package:base':

intersect, setdiff, setequal, union

Warning messages:

1: package 'fuzzyjoin' was built under R version 3.4.4

2: package 'data.table' was built under R version 3.4.4

```
> |
```

Environment History Connections

Import Dataset List

Global Environment

Functions

Flux_re...	function (input_neg...	
mmf	function (x, y)	
msMatch	function (mzFile, r...	
ref_13C...	function (refInput,...	
ref_13C...	function (refInput,...	
refLibN...	function (refInput)	
refLibP...	function (refInput)	
resultw...	function (inputFile...	
resultw...	function (inputFile...	
Sgrade	function (inputResu...	

5:118 (Top Level) R Script

Files Plots Packages Help Viewer


```

install.packages(c("fuzzyjoin", "data.table", "dplyr"))

Pah11_lipid <- Flux_result("C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_neg.csv",
  "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_pos.csv",
  "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718PahLipid12CREF.csv",
  score = 0.8)

```

You can also change the score to screen the features you want, the default one is "0.8".

```

~/
"C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_pos.csv",
"C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718PahLipid12CREF.csv")

> source('~/.R/hhuang/050618_fluxSearch_0.5/lipidFluxSearch_functions_0.5.1.R')
> Pah11_lipid <- Flux_result("C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_neg.csv",
+                           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_pos.csv",
+                           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718PahLipid12CREF.csv")
> view(Pah11_lipid)
>

```

Environment

History

Connections

Import Dataset

Global Environment

Data

Pah11_lipid

2755 obs. of 18 variables

Functions

Flux_result

function (input_negative, input_positive, referInput

mmf

function (x, y)

msMatch

function (mzFile, refFile)

ref_13C_neg

function (refInput, refoutput)

ref_13C_pos

function (refInput, refoutput)

refLibNeg_ls

function (refInput)

refLibPos_ls

function (refInput)

resultwrap_neg

function (inputFile_neg, refInput)

resultwrap_pos

function (inputFile_pos, refInput)

Sgrade

function (inputResult)

```
1 install.packages(c("fuzzyjoin", "data.table", "dplyr"))
2
3 Pah11_lipid <- Flux_result("C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/11
4 "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/11
5 "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/11
```

Highlight, and "Run"
Wait a few minutes, you will get a list
of your result

```
~/
xample/030718Pah11_neg.csv",
"C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/0
30718Pah11_pos.csv",
"C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/0
30718PahLipid12CREf.csv")

> source('~\\hhuang\\050618_fluxSearch_0.5\\lipidFluxSearch_functions_0.5.1.R')
> Pah11_lipid <- Flux_result("C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_
0.5/lipidExample/030718Pah11_neg.csv",
+ "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_
0.5/lipidExample/030718Pah11_pos.csv",
+ "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_
0.5/lipidExample/030718PahLipid12CREf.csv")
> |
```

Environment	History	Connections
Import Dataset		
Global Environment		
Data		
Pah11_lipid	2755 obs. of 18 variables	
Functions		
Flux_result	function (input_negative, input_positive, referInput, s...	
mmf	function (x, y)	
msMatch	function (mzFile, refFile)	
ref_13C_neg	function (refInput, refOutput)	
ref_13C_pos	function (refInput, refOutput)	
refLibNeg_ls	function (refInput)	
refLibPos_ls	function (refInput)	
resultwrap_neg	function (inputFile_neg, refInput)	
resultwrap_pos	function (inputFile_pos, refInput)	
Sgrade	function (inputResult)	

FileEditCodeViewPlotsSessionBuildDebugProfileToolsHelp

Go to file/function

Addins

Project: (None)

ConsoleTerminal

```
~/
"C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/0
30718Pah11_pos.csv",
"C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/0
30718PahLipid12CREF.csv")

> source('~\hhuang\050618_fluxSearch_0.5\lipidFluxSearch_functions_0.5.1.R')
> Pah11_lipid <- Flux_result("C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_
0.5/lipidExample/030718Pah11_neg.csv",
+ "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_
0.5/lipidExample/030718Pah11_pos.csv",
+ "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_
0.5/lipidExample/030718PahLipid12CREF.csv")
> view(Pah11_lipid)
> |
```

EnvironmentHistoryConnections

Import Dataset

Global Environment

Data

Pah11_lipid

2755 obs. of 18 variables

Functions

Flux_result

function (input_negative, input_positive, referInput, s...

mmf

function (x, y)

msMatch

function (mzFile, refFile)

ref_13C_neg

function (refInput, refoutput)

ref_13C_pos

function (refInput, refoutput)

refLibNeg_ls

function (refInput)

refLibPos_ls

function (refInput)

resultwrap_neg

function (inputFile_neg, refInput)

resultwrap_pos

function (inputFile_pos, refInput)

Sgrade

function (inputResult)

lph11_lipid

lipidFluxSearch_functions_0.5.1.R

Filter

	mz1	rt1	Intensity	mz2	rt2	Lipid	fattyAcid	lipidClass	lipidF
147	742.5399	22.010500	13981924.00	742.5399	22.009742	PE(18:1/18:1)-H	(18:1/18:1)	PE	C4
1468	462.2995	9.008433	739520.94	462.2995	9.001202	LPE(18:1p)-H	(18:1p)	LPE	C2
179	700.5292	22.750833	12251509.00	700.5293	22.745778	PE(16:0p/18:1)-H	(16:0p/18:1)	PE	C3
306	768.5552	22.973333	7437574.50	768.5552	22.964694	PE(18:0/20:3)-H	(18:0/20:3)	PE	C4
378	728.5605	24.394667	6414302.00	728.5605	24.383658	PE(18:0p/18:1)-H	(18:0p/18:1)	PE	C4
638	760.5142	20.932333	3131829.50	760.5143	20.932706	PS(16:0/18:1)-H	(16:0/18:1)	PS	C4
244	776.5453	19.969000	10498442.00	776.5452	19.957305	PC(16:0/16:1)+HCOO	(16:0/16:1)	PC	C4
2334	538.3155	5.472100	153215.69	538.3155	5.474729	LPC(16:1)+HCOO	(16:1)	LPC	C2
266	778.5610	21.445667	8612351.00	778.5611	21.452028	PC(16:0/16:0)+HCOO	(16:0/16:0)	PC	C4
432	774.5441	20.932333	5455769.00	774.5443	20.939675	PE(18:1p/22:5)-H	(18:1p/22:5)	PE	C4
291	716.5242	21.932167	7803598.00	716.5241	21.945243	PE(16:0/18:1)-H	(16:0/18:1)	PE	C3
1845	886.6551	24.888833	335632.53	886.6550	24.902252	PC(18:1/22:1)+HCOO	(18:1/22:1)	PC	C4
92	885.5506	20.685167	17844100.00	885.5505	20.682209	PI(18:0/20:4)-H	(18:0/20:4)	PI	C4
2296	524.2995	9.527583	157793.80	524.2994	9.507010	LPS(18:0)-H	(18:0)	LPS	C2
1349	824.5451	18.493667	963580.06	824.5451	18.467669	PC(16:1/20:4)+HCOO	(16:1/20:4)	PC	C4
937	774.5322	19.370000	1896691.00	774.5322	19.343262	PC(16:0/16:2)+HCOO	(16:0/16:2)	PC	C4
282	726.5448	22.824833	7957691.00	726.5447	22.849450	PE(18:1p/18:1)-H	(18:1p/18:1)	PE	C4
2597	509.2885	7.233267	80667.59	509.2886	7.238593	LPG(18:1)-H	(18:1)	LPG	C2
2495	450.2629	5.818633	110861.34	450.2630	5.797116	LPE(16:1)-H	(16:1)	LPE	C2
80	788.5458	22.473833	18722590.00	788.5460	22.501573	PS(18:0/18:1)-H	(18:0/18:1)	PS	C4
868	858.6235	23.288500	2043204.38	858.6233	23.317062	PC(20:1/18:1)+HCOO	(20:1/18:1)	PC	C4
224	857.6761	25.096333	11309874.00	857.6760	25.064706	SM(d16:0/26:2)+HCOO	(d16:0/26:2)	SM	C4
1104	698.5134	21.103833	1489132.62	698.5134	21.137712	PE(18:1p/16:1)-H	(18:1p/16:1)	PE	C3
1149	800.5455	19.170667	1449120.00	800.5458	19.161588	PC(16:2/18:1)+HCOO	(16:2/18:1)	PC	C4
2429	690.5076	22.143333	129230.17	690.5078	22.164878	PE(16:0/16:0)-H	(16:0/16:0)	PE	C3
2040	833.5183	18.817000	255808.11	833.5181	18.838139	PI(16:1/18:1)-H	(16:1/18:1)	PI	C4
1264	780.5913	25.422000	1079259.00	780.5916	25.410766	PE(18:0p/22:3)-H	(18:0p/22:3)	PE	C4

Showing 1 to 29 of 2,755 entries

FilesPlotsPackagesHelpViewer

Type here to search

4:12 PM

5/16/2018

```
1 install.packages(c("fuzzyjoin", "data.table", "dplyr"))
2
3 Pah11_lipid <- Flux_result("C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_neg.csv",
4                           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_pos.csv",
5                           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718PahLipid12CREF.csv",
6                           score = 0.8)
7
8 write.csv(Pah11_lipid,
9           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718PahLipid.csv")
```

Output your result as CSV file, using the “write.csv(...)” function.

```
> source('~\\hhuang\\050618_fluxSearch_0.5\\lipidFluxSearch_functions_0.5.1.R')
> Pah11_lipid <- Flux_result("C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_neg.csv",
+                           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718Pah11_pos.csv",
+                           "C:/Users/hhuang4/Documents/hhuang/050618_fluxSearch_0.5/lipidExample/030718PahLipid12CREF.csv")
> view(Pah11_lipid)
> |
```

Environment History Connections

Import Dataset List

Global Environment

Data

Pah11_lipid 2755 obs. of 18 variables

Functions

Flux_result	function (input_negative, ...)	
mmf	function (x, y)	
msMatch	function (mzFile, refFile)	
ref_13C_neg	function (refInput, refout...)	
ref_13C_pos	function (refInput, refout...)	
refLibNeg_...	function (refInput)	
refLibPos_...	function (refInput)	
resultwrap...	function (inputFile_neg, r...	
resultwrap...	function (inputFile_pos, r...	
Sgrade	function (inputResult)	