

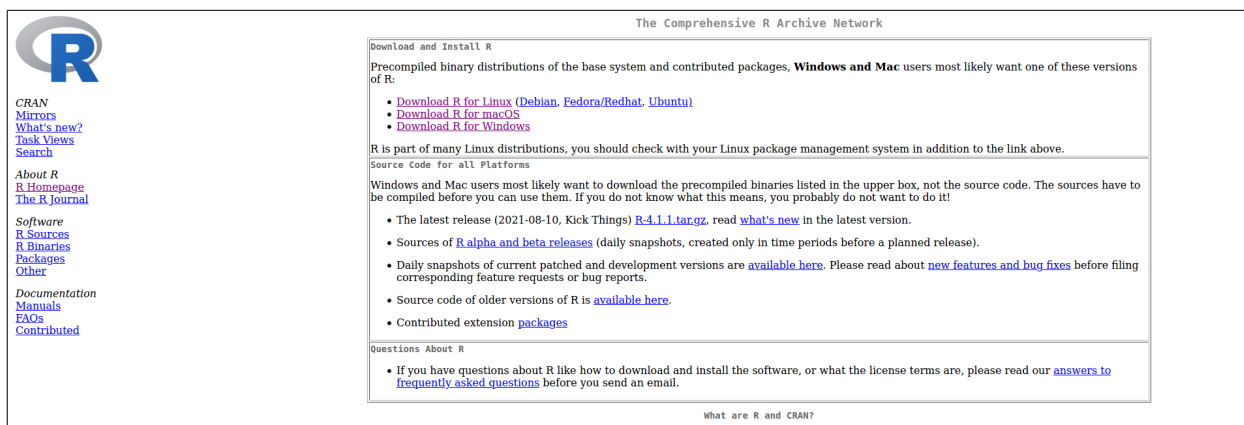
Lipidomics Data Analysis Workshop

Date/time: September 23, 2021, 3:00 pm – 4:30 pm
Where: SRB 120

- I. The data analysis makes use of an R script. To run this R script on your own computer you will need R and RStudio installed. If you would like to analyze the sample data during the workshop, then the following software will need to be installed:

A. Download R from <https://rweb.crmda.ku.edu/cran/>

- i. Choose your operating system



The screenshot shows the CRAN website with the 'Download and Install R' section. It provides instructions for downloading R on various operating systems, including Linux, macOS, and Windows. It also mentions source code for all platforms and provides links to frequently asked questions.

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Download and Install R

Precompiled binary distributions of the base system and contributed packages, **Windows and Mac** users most likely want one of these versions of R:

- [Download R for Linux \(Debian, Fedora/Redhat, Ubuntu\)](#)
- [Download R for macOS](#)
- [Download R for Windows](#)

R is part of many Linux distributions, you should check with your Linux package management system in addition to the link above.

Source Code for all Platforms

Windows and Mac users most likely want to download the precompiled binaries listed in the upper box, not the source code. The sources have to be compiled before you can use them. If you do not know what this means, you probably do not want to do it!

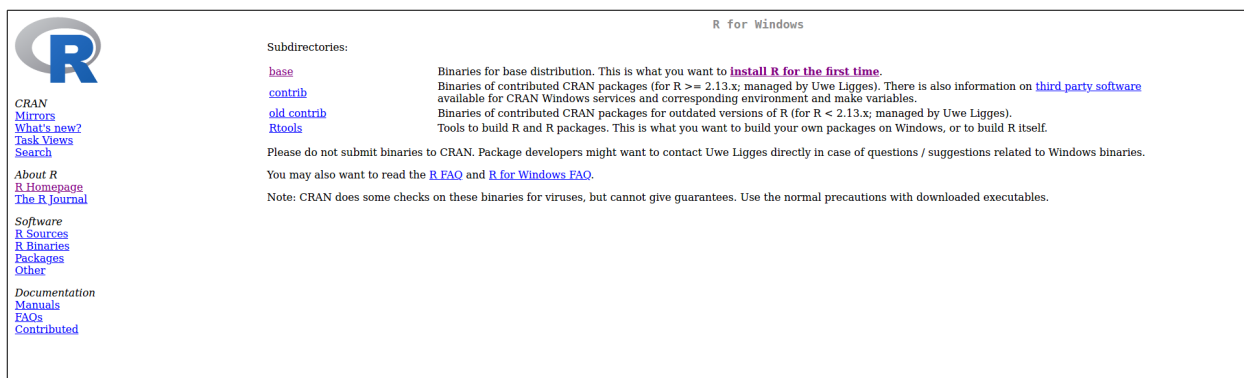
- The latest release (2021-08-10, Kick Things) [R4.1.1.tar.gz](#), read [what's new](#) in the latest version.
- Sources of [R alpha and beta releases](#) (daily snapshots, created only in time periods before a planned release).
- Daily snapshots of current patched and development versions are [available here](#). Please read about [new features](#) and [bug fixes](#) before filing corresponding feature requests or bug reports.
- Source code of older versions of R is [available here](#).
- Contributed extension [packages](#)

Questions About R

- If you have questions about R like how to download and install the software, or what the license terms are, please read our [answers to frequently asked questions](#) before you send an email.

What are R and CRAN?

- ii. Choose 'base'



The screenshot shows the CRAN website with the 'R for Windows' section. It provides instructions for downloading R on Windows, including links to the base distribution, contributed packages, and tools to build R and R packages. It also mentions that CRAN does some checks on these binaries for viruses, but cannot give guarantees.

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R for Windows

Subdirectories:

- [base](#)
- [contrib](#)
- [old.contrib](#)
- [Rtools](#)

Binaries for base distribution. This is what you want to **install R for the first time**.
Binaries of contributed CRAN packages (for R >= 2.13.x; managed by Uwe Ligges). There is also information on [third party software](#) available for CRAN Windows services and corresponding environment and make variables.
Binaries of contributed CRAN packages for outdated versions of R (for R < 2.13.x; managed by Uwe Ligges).
Tools to build R and R packages. This is what you want to build your own packages on Windows, or to build R itself.

Please do not submit binaries to CRAN. Package developers might want to contact Uwe Ligges directly in case of questions / suggestions related to Windows binaries.

You may also want to read the [R FAQ](#) and [R for Windows FAQ](#).

Note: CRAN does some checks on these binaries for viruses, but cannot give guarantees. Use the normal precautions with downloaded executables.

iii. Click on 'Download R 4.1.1 for Windows' and follow install instructions



CRAN

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About R

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Documentation

[Manuals](#)

[FAQs](#)

[Contributed](#)

R-4.1.1 for Windows (32/64 bit)

[Download R 4.1.1 for Windows](#) (86 megabytes, 32/64 bit)

[Installation and other instructions](#)

[New features in this version](#)

If you want to double-check that the package you have downloaded matches the package distributed by CRAN, you can compare the [md5sum](#) of the .exe to the [fingerprint](#) on the master server. You will need a version of md5sum for windows: both [graphical](#) and [command line versions](#) are available.

Frequently asked questions

- [Does R run under my version of Windows?](#)
- [How do I update packages in my previous version of R?](#)
- [Should I run 32-bit or 64-bit R?](#)

Please see the [R FAQ](#) for general information about R and the [R Windows FAQ](#) for Windows-specific information.

Other builds

- Patches to this release are incorporated in the [r-patched snapshot build](#).
- A build of the development version (which will eventually become the next major release of R) is available in the [r-devel snapshot build](#).
- [Previous releases](#)

Note to webmasters: A stable link which will redirect to the current Windows binary release is [<CRAN MIRROR>/bin/windows/base/release.html](#).


Last change: 2021-08-10

B. Download and Install RStudio from

<https://www.rstudio.com/products/rstudio/download/>

RStudio Desktop 1.4.1717 - Release Notes

1. Install R. RStudio requires R 3.0.1+.
2. Download RStudio Desktop. Find your operating system in the table below.



All Installers

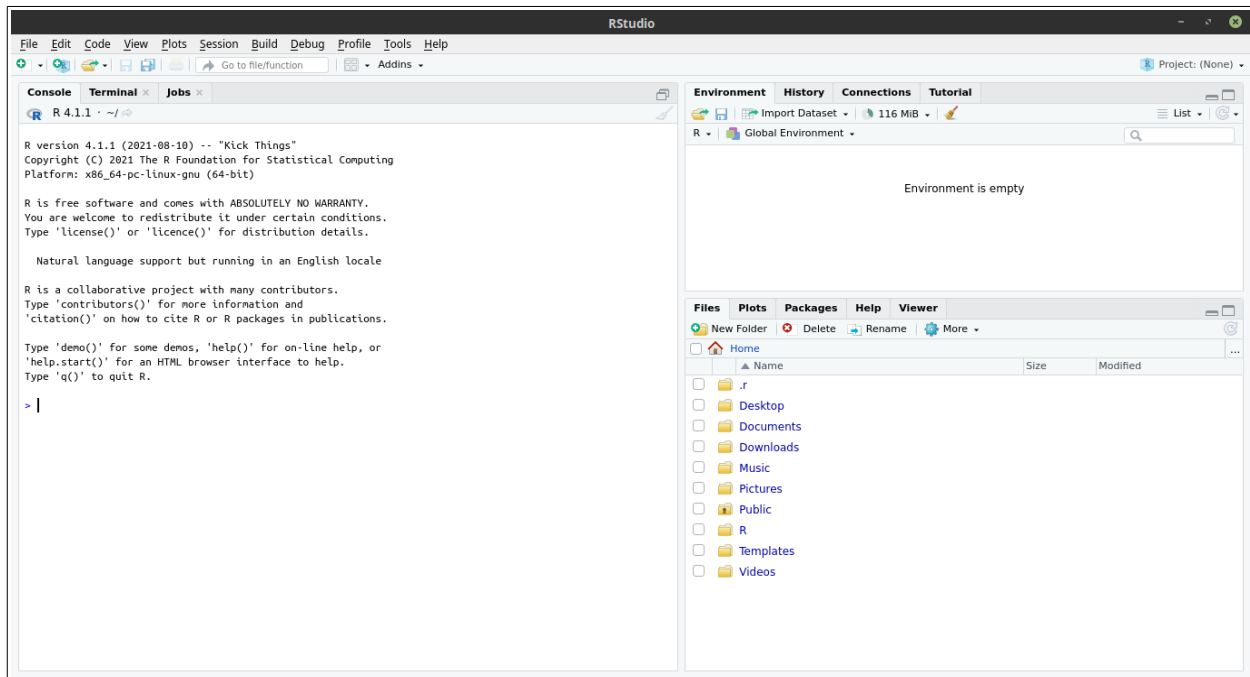
Linux users may need to [import RStudio's public code-signing key](#) prior to installation, depending on the operating system's security policy.

RStudio requires a 64-bit operating system. If you are on a 32 bit system, you can use an [older version of RStudio](#).

OS	Download	Size	SHA-256
Windows 10	RStudio-1.4.1717.exe	156.18 MB	71b36e64
macOS 10.14+	RStudio-1.4.1717.dmg	203.06 MB	2cf2549d
Ubuntu 18/Debian 10	rstudio-1.4.1717-amd64.deb	122.51 MB	e27b2645
Fedora 19/Red Hat 7	rstudio-1.4.1717-x86_64.rpm	138.42 MB	648e2be0
Fedora 28/Red Hat 8	rstudio-1.4.1717-x86_64.rpm	138.39 MB	c76f620a
Debian 9	rstudio-1.4.1717-amd64.deb	123.29 MB	e4ea3a60
OpenSUSE 15	rstudio-1.4.1717-x86_64.rpm	123.15 MB	e69d55db

C. Install 'tidyverse' and 'data.table' R libraries

i. Open RStudio



ii. In the console panel type the following and then press Enter:

```
install.packages('tidyverse')
```

```
R version 4.1.1 (2021-08-10) -- "Kick Things"
Copyright (C) 2021 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

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.

Natural language support but running in an English locale

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.

> install.packages('tidyverse')
```

a) Note: you will see many packages install that will be used by R for data and statistical analysis. This will take several minutes.

iii. Next, in the console type the following and then press Enter:

```
install.packages('data.table')
```

iv. Test to make sure libraries have successfully installed by typing the following in the console and pressing Enter after each:

```
library(tidyverse)
```

```
library(data.table)
```

```
> library(tidyverse)
— Attaching packages — tidyverse 1.3.1 —
✓ ggplot2 3.3.5   ✓ purrr 0.3.4
✓ tibble 3.1.4   ✓ dplyr 1.0.7
✓ tidyr 1.1.3    ✓ stringr 1.4.0
✓ readr 2.0.1    ✓ forcats 0.5.1
— Conflicts — tidyverse_conflicts() —
x dplyr::filter() masks stats::filter()
x dplyr::lag() masks stats::lag()
> library(data.table)
data.table 1.14.0 using 2 threads (see ?getDTthreads). Latest news: r-datatable.com

Attaching package: 'data.table'

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

  between, first, last

The following object is masked from 'package:purrr':

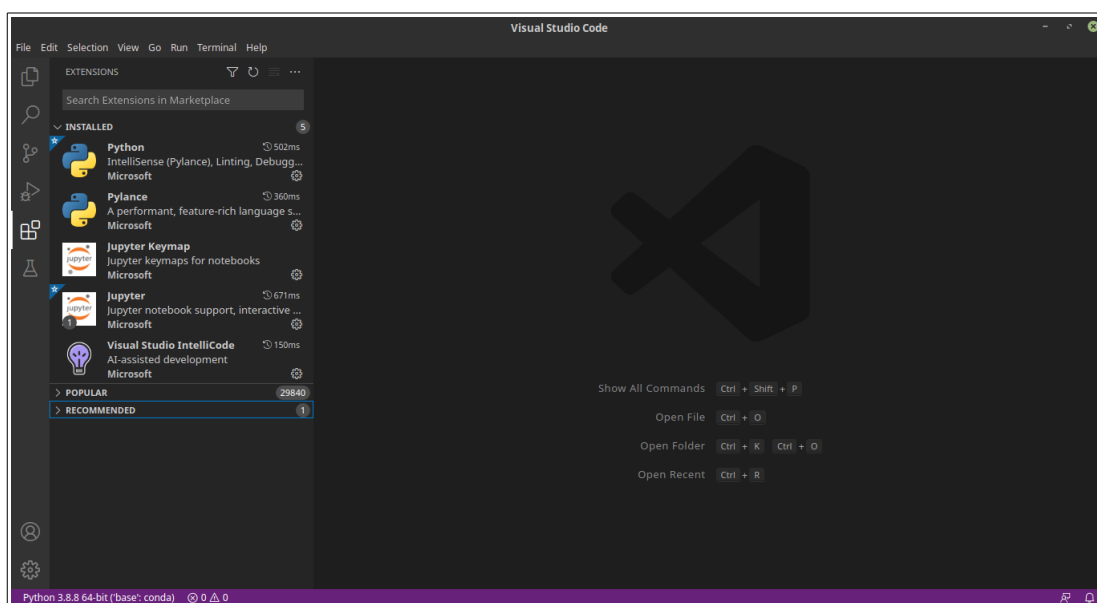
  transpose
```

a) Note: If errors occur, you may need to determine if you have missing packages.

D. Download the zip file containing the R scripts and sample data we will be using from [here](#). This is the data we will use to practice the data analysis workflow.

II. There are a few helpful Python scripts that were made and helpful for producing MRM tables or calculating lipid molecular masses and their adduct forms. This section is **OPTIONAL** and not required for the workshop, but if you'd like to make use of these Python scripts the following software is recommended:

- A. Anaconda is a useful suite of data analysis tools, many of which use Python3. There are two different flavors you can download, either the full suite called 'Anaconda' or the pared down version 'Miniconda'. The former requires a few Gb of space and will take some time to install while the latter will be the minimal install and require additional steps afterwards. Either version can be installed from <https://docs.conda.io/projects/conda/en/latest/user-guide/install/index.html>. Follow the install instructions there.
- i. Note: If you chose to install Miniconda, be sure to also install the Python libraries for 'Numpy', 'Pandas', and 'Matplotlib'. Others may be required.
- B. Microsoft's Visual Studio Code is an integrated development environment (IDE) that can be used for virtually any type of code. Here it is quite useful for Python3 and data analysis and can be downloaded from <https://code.visualstudio.com/>.
- i. Note: To make the most use of Python3 within Visual Studio Code, also be sure to install the internal apps: 'Python', 'Pylance', 'Jupyter', 'Visual Studio Intellicode'. These apps will help autocomplete commands and allow for data analysis within the IDE.



III. Below are a list of useful resources and software for lipidomics, plant lipid metabolism, and data analysis. These are for your future reference.

A. R resources

- i. R: <https://www.r-project.org/>
 - a) (additional libraries: tidyverse & data.table)
- ii. Rstudio: <https://www.rstudio.com/products/rstudio/>
- iii. R for Data Science (online ebook): <https://r4ds.had.co.nz/index.html>
- iv. Tidyverse library: <https://www.tidyverse.org/>
- v. Data.Table library: <https://cran.r-project.org/web/packages/data.table/vignettes/datatable-intro.html>
- vi. W3: <https://www.w3schools.com/r/default.asp>

B. Python Resources

- i. Anaconda: <https://www.anaconda.com/>
- ii. Visual Studio Code: <https://code.visualstudio.com/>
 - a) (internal apps: Python, Pylance, Jupyter, Visual Studio Intellicode)
- iii. Python Data Science Handbook (online ebook):
<https://jakevdp.github.io/PythonDataScienceHandbook/>
- iv. Numpy (included with Anaconda): <https://numpy.org/>
- v. Pandas (included with Anaconda): <https://pandas.pydata.org/>
- vi. Matplotlib (included with Anaconda): <https://matplotlib.org/>
- vii. W3: <https://www.w3schools.com/python/default.asp>

C. mMass (viewing spectra/chromatogram from .txt file): <http://www.mmass.org/>

D. MarvinSketch (chemical drawing): <https://chemaxon.com/products/marvin>

E. Metaboanalyst (statistical analysis): <https://www.metaboanalyst.ca/>

F. Lipid Metabolic Background Information

- i. AOCS Lipid Library: <https://lipidlibrary.aocs.org/>
- ii. ARALIP: The Arabidopsis Acyl-Lipid Metabolism Website:
<http://aralip.plantbiology.msu.edu/about>
- iii. Acyl-Lipid Metabolism: <https://doi.org/10.1199/tab.0133>
- iv. LIPID MAPS: <https://www.lipidmaps.org/>