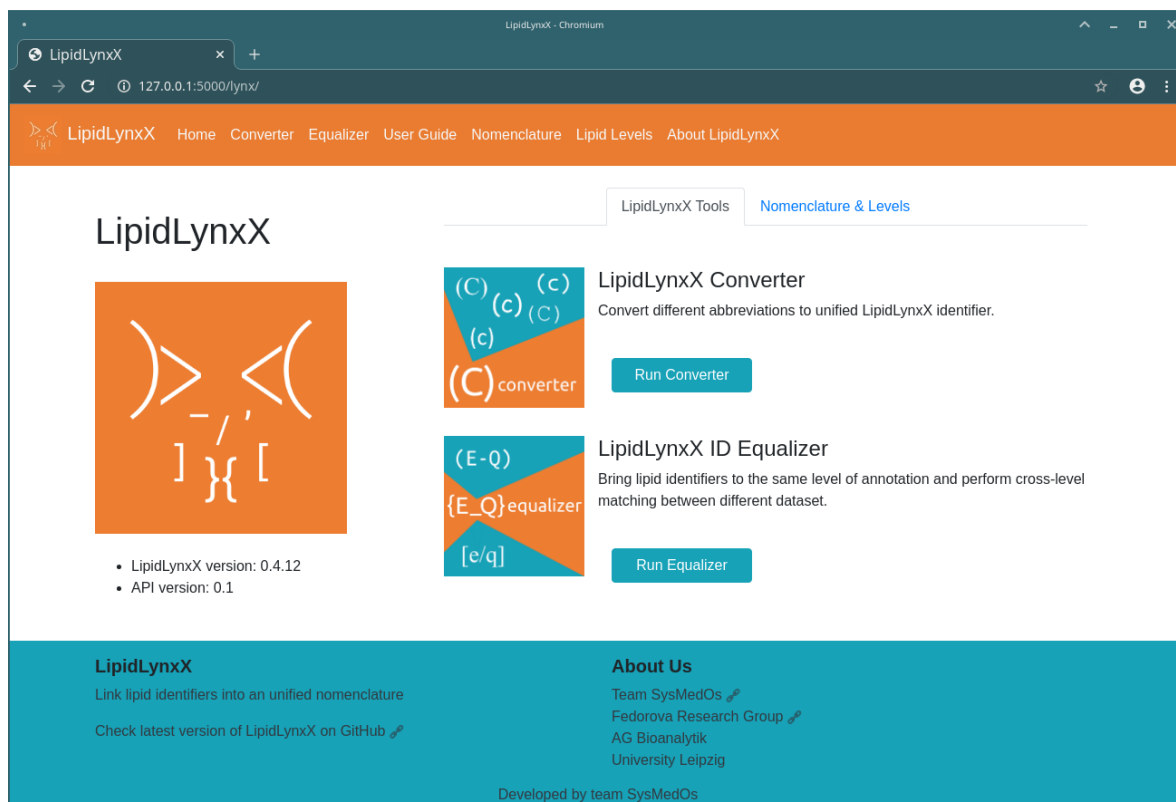


# LipidLynxX User Guide



## This user guide is designed for:

- LipidLynxX version: v0.4.12
- API version: v0.1

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## How to install LipidLynxX




### Install from exe version for Windows 10

Please get the latest version from LipidLynxX repository on GitHub using the link below:

<https://github.com/SysMedOs/LipidLynxX/releases>

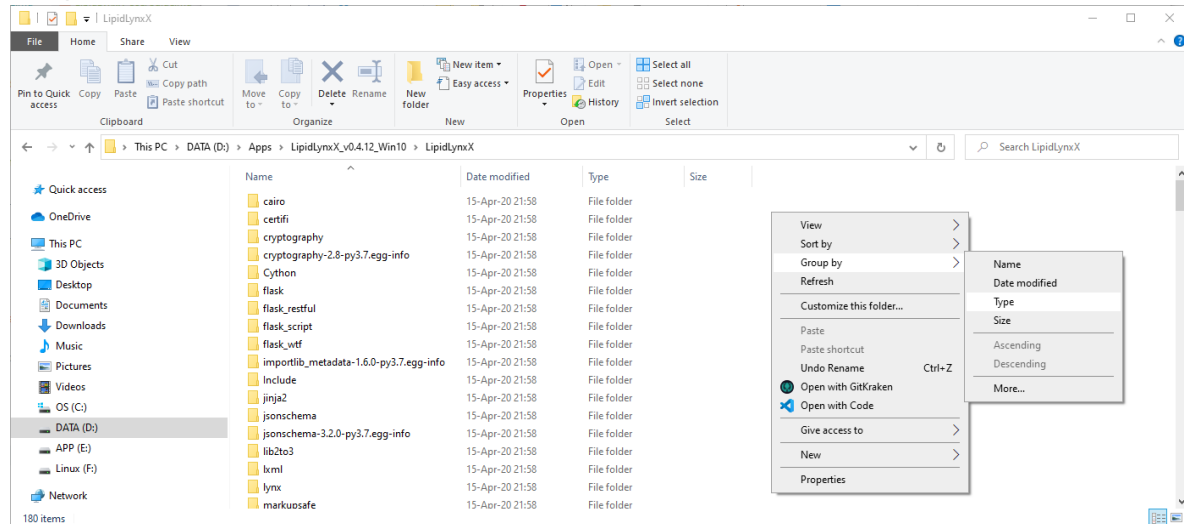
In each release, there is always an `Assets` section. Please download the Windows version in `.zip` format (usually around 350 MB).

## Assets 3

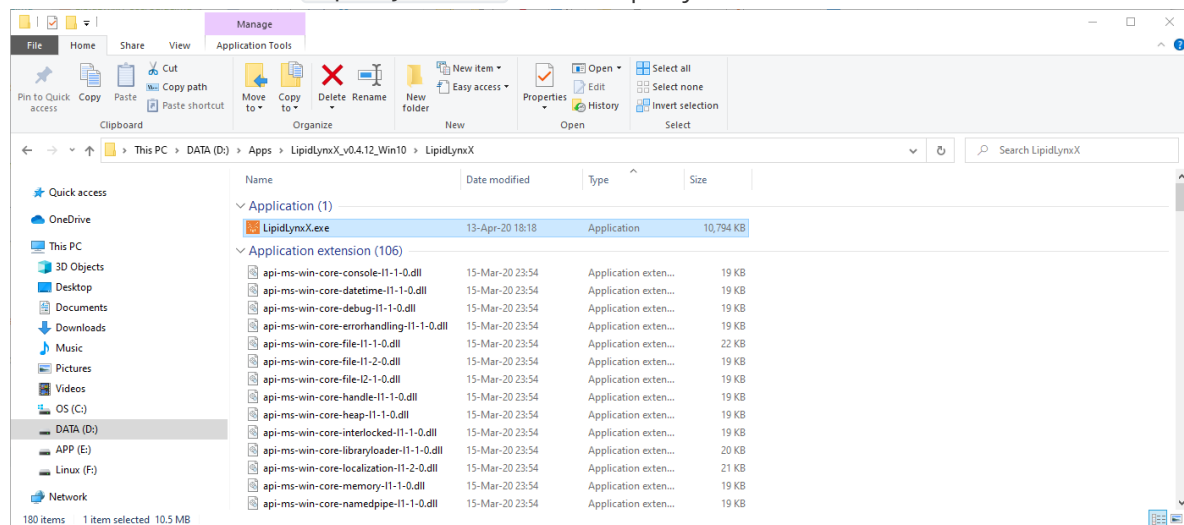
 <b>LipidLynxX_v0.4.12_Win10.zip</b> 333 MB
 <b>Source code (zip)</b>
 <b>Source code (tar.gz)</b>

When the file is successfully downloaded, you can unzip it to any folder .e.g

D:/Apps/LipidLynxX. Open the folder of LipidLynxX and you can find the **LipidLynxx.exe** by using **right click -> Group by -> Type**



You can double click on **LipidLynxx.exe** to start LipidLynxX



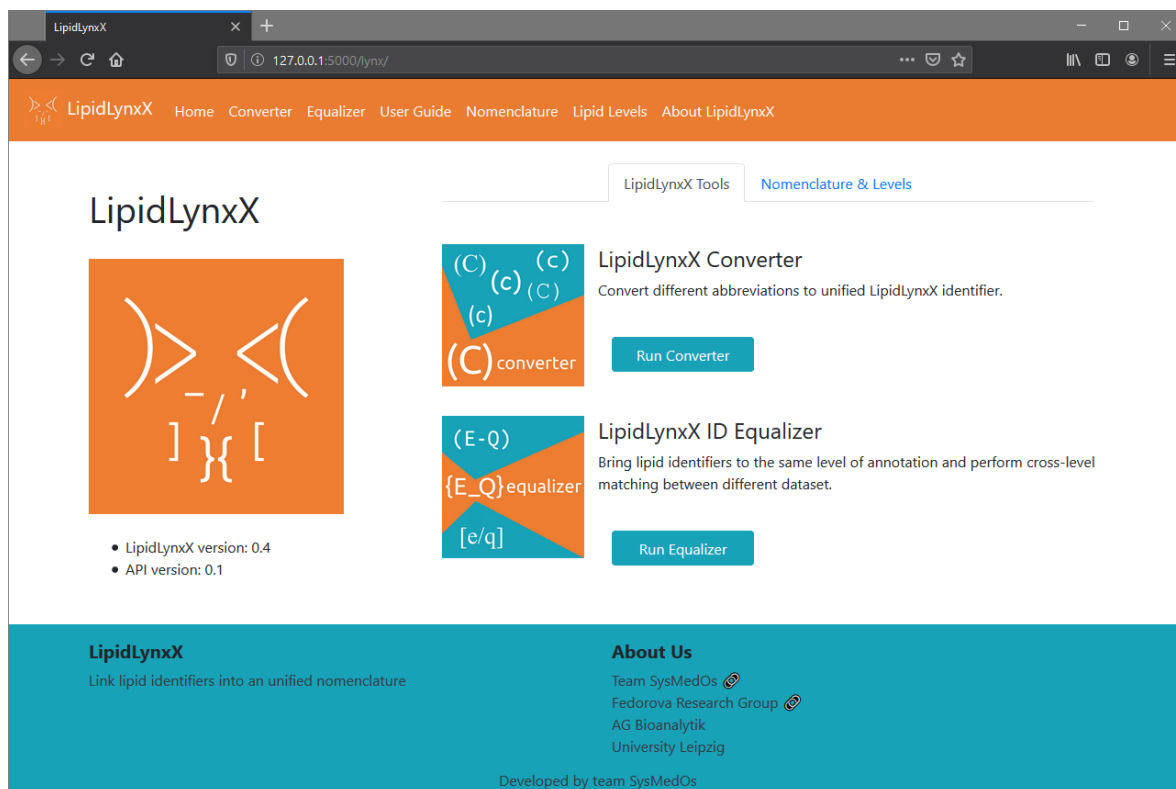
Your antivirus may block it first and shows a blue frame. After virus checking finished, it may have some error message. Close all warnings and this command prompt window.

```
D:\Apps\LipidLynxX_v0.4.12_Win10\LipidLynxX\LipidLynxX.exe
x.V0): 'ST', regex.Regex('ST', flags=regex.V0): 'ST'}}, 'RESIDUES': {'RESIDUE': {'ORDER': ['LINK', 'NUM_C', 'DB_SEPARATOR', 'NUM_DB', 'O_SEPARATOR', 'NUM_O', 'MOD_BRACKET_LEFT', 'SUM_MODS', 'MOD_BRACKET_RIGHT'], 'OPTIONAL': ['LINK', 'DB', 'O_SEPARATOR', 'NUM_O', 'MOD_BRACKET_LEFT', 'SUM_MODS', 'MOD_BRACKET_RIGHT'], 'REPEAT': {'SUM_MODS': [0, 10]}, 'LINK': '[OP]-[C][mdt][h]', 'NUM_C': '[0-9]{1,2}', 'DB_SEPARATOR': ':', 'NUM_DB': '[1,2]?[0-9]', 'O_SEPARATOR': ';', 'NUM_O': ';[1-3]?0?', 'MOD_BRACKET_LEFT': '$SEPARATORS.MOD_BRACKET_LEFT.0', 'SUM_MODS': '$MODS.SUM_MODS.0', 'MOD_BRACKET_RIGHT': '$SEPARATORS.MOD_BRACKET_LEFT.0', 'EXCEPTIONS': {'PREFIX': 'TEST'}, 'MODS': {'MOD': {'ORDER': ['MOD_COUNT', 'MOD_CV', 'SITE_BRACKET_LEFT', 'MOD_SITE', 'MOD_SITE_INFO', 'SITE_BRACKET_RIGHT'], 'OPTIONAL': ['MOD_COUNT', 'MOD_CV', 'SITE_BRACKET_LEFT', 'MOD_SITE', 'MOD_SITE_INFO', 'SITE_BRACKET_LEFT'], 'REPEAT': {'MOD': [1, 10]}, 'MOD_COUNT': '\\d?\\d?', 'MOD_CV': '([a-zA-Z]*[-0-9a-zA-Z]*)', 'SITE_BRACKET_LEFT': '$SEPARATORS.MODS_BRACKET_LEFT.0', 'MOD_SITE': '\\s?)([0-9]{1,2})', 'MOD_SITE_INFO': '([EZR])?', 'SITE_BRACKET_RIGHT': '$SEPARATORS.SITE_BRACKET_RIGHT.0', 'EXAMPLES': ['(9,12)', '(9Z,12Z)', 'OH', '2OH', 'OH(8R)', '2OH(8R,15S)'], 'SUM_MODS': {'ORDER': ['RESIDUE_BRACKET_LEFT', 'MOD', 'RESIDUE_BRACKET_RIGHT'], 'REPEAT': {'MOD_SITE': [1, 10], 'MOD_SITE_INFO': [1, 10]}, 'BRACKET_LEFT': '$SEPARATORS.BRACKET_LEFT.0', 'MOD': '$MODS.MOD.0', 'RESIDUE_BRACKET_RIGHT': '$SEPARATORS.BRACKET_RIGHT.0', 'EXAMPLES': ['(9Z)', '(9Z,12Z)', '(9OH,12OH)']}}, 'SEPARATORS': {'DB_SEPARATOR': ':', 'O_SEPARATOR': ';', 'RESIDUE_BRACKET_LEFT': '(', 'RESIDUE_BRACKET_RIGHT': ')', 'MOD_BRACKET_LEFT': '<', 'MOD_BRACKET_RIGHT': '>', 'SITE_BRACKET_LEFT': '{', 'SITE_BRACKET_RIGHT': '}', 'SQUARE_BRACKET_LEFT': '[', 'SQUARE_BRACKET_RIGHT': ']', 'SEPARATOR_LEVELS': {'B': '', 'D': '_', 'S': '/'}}}}
Apr-15@22:11:59[INFO ] Default parameters loaded successfully.
Apr-15@22:11:59[INFO ] Lynx API config loaded...
* Debugger is active!
* Debugger PIN: 275-812-030
* Running on http://127.0.0.1:5000/ (Press CTRL+C to quit)
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /lynx/ HTTP/1.1" 200 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /lynx/ HTTP/1.1" 200 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/LipidLynxX_Logo_banner.jpg HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/LipidLynxX_Logo.png HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/converter_logo.png HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/equalizer_logo.png HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/nomenclature_logo.png HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:01] "GET /favicon.ico HTTP/1.1" 404 -
```

Now click on [LipidLynxX.exe](#) again and the following command prompt window will show up without any error message.

```
D:\Apps\LipidLynxX_v0.4.12_Win10\LipidLynxX\LipidLynxX.exe
x.V0): 'ST', regex.Regex('ST', flags=regex.V0): 'ST'}}, 'RESIDUES': {'RESIDUE': {'ORDER': ['LINK', 'NUM_C', 'DB_SEPARATOR', 'NUM_DB', 'O_SEPARATOR', 'NUM_O', 'MOD_BRACKET_LEFT', 'SUM_MODS', 'MOD_BRACKET_RIGHT'], 'OPTIONAL': ['LINK', 'DB', 'O_SEPARATOR', 'NUM_O', 'MOD_BRACKET_LEFT', 'SUM_MODS', 'MOD_BRACKET_RIGHT'], 'REPEAT': {'SUM_MODS': [0, 10]}, 'LINK': '[OP]-[C][mdt][h]', 'NUM_C': '[0-9]{1,2}', 'DB_SEPARATOR': ':', 'NUM_DB': '[1,2]?[0-9]', 'O_SEPARATOR': ';', 'NUM_O': ';[1-3]?0?', 'MOD_BRACKET_LEFT': '$SEPARATORS.MOD_BRACKET_LEFT.0', 'SUM_MODS': '$MODS.SUM_MODS.0', 'MOD_BRACKET_RIGHT': '$SEPARATORS.MOD_BRACKET_LEFT.0', 'EXCEPTIONS': {'PREFIX': 'TEST'}, 'MODS': {'MOD': {'ORDER': ['MOD_COUNT', 'MOD_CV', 'SITE_BRACKET_LEFT', 'MOD_SITE', 'MOD_SITE_INFO', 'SITE_BRACKET_RIGHT'], 'OPTIONAL': ['MOD_COUNT', 'MOD_CV', 'SITE_BRACKET_LEFT', 'MOD_SITE', 'MOD_SITE_INFO', 'SITE_BRACKET_LEFT'], 'REPEAT': {'MOD': [1, 10]}, 'MOD_COUNT': '\\d?\\d?', 'MOD_CV': '([a-zA-Z]*[-0-9a-zA-Z]*)', 'SITE_BRACKET_LEFT': '$SEPARATORS.MODS_BRACKET_LEFT.0', 'MOD_SITE': '\\s?)([0-9]{1,2})', 'MOD_SITE_INFO': '([EZR])?', 'SITE_BRACKET_RIGHT': '$SEPARATORS.SITE_BRACKET_RIGHT.0', 'EXAMPLES': ['(9,12)', '(9Z,12Z)', 'OH', '2OH', 'OH(8R)', '2OH(8R,15S)'], 'SUM_MODS': {'ORDER': ['RESIDUE_BRACKET_LEFT', 'MOD', 'RESIDUE_BRACKET_RIGHT'], 'REPEAT': {'MOD_SITE': [1, 10], 'MOD_SITE_INFO': [1, 10]}, 'BRACKET_LEFT': '$SEPARATORS.BRACKET_LEFT.0', 'MOD': '$MODS.MOD.0', 'RESIDUE_BRACKET_RIGHT': '$SEPARATORS.BRACKET_RIGHT.0', 'EXAMPLES': ['(9Z)', '(9Z,12Z)', '(9OH,12OH)']}}, 'SEPARATORS': {'DB_SEPARATOR': ':', 'O_SEPARATOR': ';', 'RESIDUE_BRACKET_LEFT': '(', 'RESIDUE_BRACKET_RIGHT': ')', 'MOD_BRACKET_LEFT': '<', 'MOD_BRACKET_RIGHT': '>', 'SITE_BRACKET_LEFT': '{', 'SITE_BRACKET_RIGHT': '}', 'SQUARE_BRACKET_LEFT': '[', 'SQUARE_BRACKET_RIGHT': ']', 'SEPARATOR_LEVELS': {'B': '', 'D': '_', 'S': '/'}}}}
Apr-15@22:11:59[INFO ] Default parameters loaded successfully.
Apr-15@22:11:59[INFO ] Lynx API config loaded...
* Debugger is active!
* Debugger PIN: 275-812-030
* Running on http://127.0.0.1:5000/ (Press CTRL+C to quit)
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /lynx/ HTTP/1.1" 200 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /lynx/ HTTP/1.1" 200 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/LipidLynxX_Logo_banner.jpg HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/LipidLynxX_Logo.png HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/converter_logo.png HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/equalizer_logo.png HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:00] "GET /static/images/nomenclature_logo.png HTTP/1.1" 304 -
127.0.0.1 - - [15/Apr/2020 22:12:01] "GET /favicon.ico HTTP/1.1" 404 -
```

A web browser window will start automatically and load the LipidLynxX local web service at: <http://127.0.0.1:5000/lynx/> Please make sure you have Chrome or Firefox installed.



If windows internet explorer or Microsoft Edge browser started by default, please start Chrome or Firefox manually and visit <http://127.0.0.1:5000/lynx/>

Now you have LipidLynxX installed successfully.

Please leave the LipidLynxX command prompt window on during the run. If you accidentally close the web page of LipidLynxX, you can always visit <http://127.0.0.1:5000/lynx/> to get back to LipidLynxX.

If you want to quit LipidLynxX, just close the LipidLynxX command prompt window, and then the LipidLynxX at <http://127.0.0.1:5000/lynx/> will be switched off. Please make sure you saved all your output files before closing the LipidLynxX command prompt window.

## Install from source code

Please make sure you have `git` installed.

You can use python 3.7.6 directly, using virtual environment is strongly recommended. In this tutorial, `conda` from `anaconda` or `miniconda` is used. Please find the installation guide of conda for your system on the following link: <https://docs.anaconda.com/anaconda/install/>

Following commands can be used on platforms including Linux, macOS, and Windows 10. The screenshots are mainly taken on Ubuntu Linux 18.04 LTS with zsh, however, it may have different style of terminal window display on your system, but the commands and the main output should stay the same cross platforms.

After successful installation of `git` and `conda`, you can clone the LipidLynxX source code to your disk. e.g. on Ubuntu Linux 18.04 LTS with zsh:

```
git clone --depth=50 --branch=master https://github.com/SysMedOs/LipidLynxX.git
LipidLynxX
```

```
Terminal - ni@bbzpcagho12: ~
File Edit View Terminal Tabs Help
> git clone --depth=50 --branch=master https://github.com/SysMed0s/LipidLynxX.git LipidLynxX
Cloning into 'LipidLynxX'...
remote: Enumerating objects: 133, done.
remote: Counting objects: 100% (133/133), done.
remote: Compressing objects: 100% (102/102), done.
remote: Total 2138 (delta 44), reused 90 (delta 24), pack-reused 2005
Receiving objects: 100% (2138/2138), 8.34 MiB | 10.81 MiB/s, done.
Resolving deltas: 100% (1432/1432), done.
```

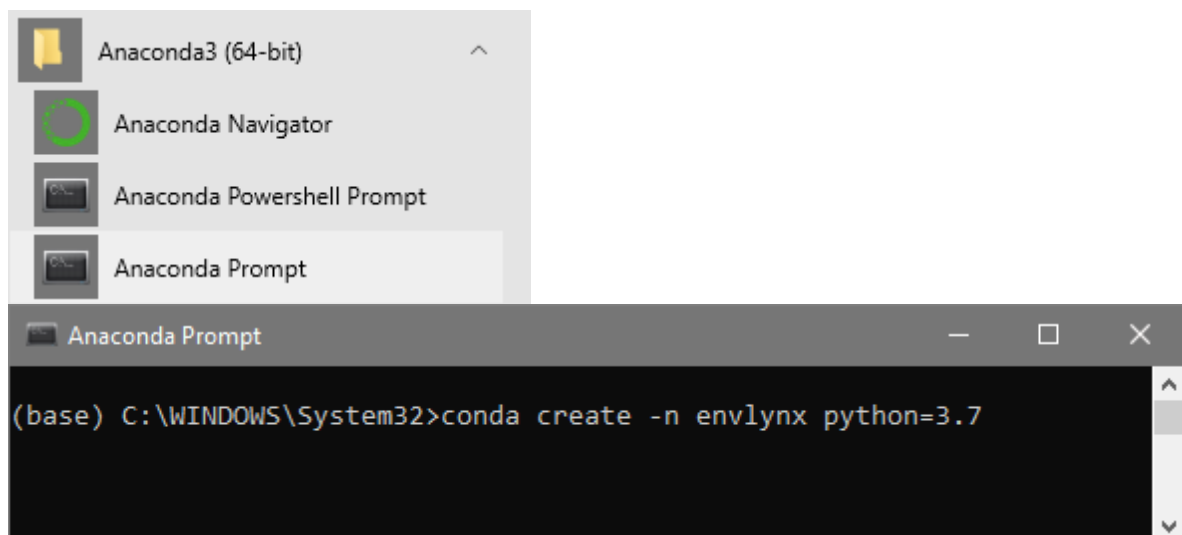
Now you can create a virtual environment for LipidLynxX. For Windows users, please use the `Anaconda Prompt` instead of `CommandLine Prompt` or `Power Shell` here a virtual environment named `envlynx` is created. You might have to type `y` for `enter` to confirm the creation of this virtual environment.

```
conda create -n envlynx python=3.7
```

e.g. on Ubuntu Linux 18.04 LTS with zsh:

```
Terminal - ni@bbzpcagho12: ~
File Edit View Terminal Tabs Help
> git clone --depth=50 --branch=master https://github.com/SysMed0s/LipidLynxX.git LipidLynxX
Cloning into 'LipidLynxX'...
remote: Enumerating objects: 133, done.
remote: Counting objects: 100% (133/133), done.
remote: Compressing objects: 100% (102/102), done.
remote: Total 2138 (delta 44), reused 90 (delta 24), pack-reused 2005
Receiving objects: 100% (2138/2138), 8.34 MiB | 10.81 MiB/s, done.
Resolving deltas: 100% (1432/1432), done.
> conda create -n envlynx python=3.7
```

For Windows users:



You can then activate the virtual environment created above. Notice that the indicator of your python environment will be changed from `anconda`, `base`, or `miniconda` to the name of the virtual environment created above (`envlynx`). e.g. on Ubuntu Linux 18.04 LTS with zsh:

A terminal window titled "Terminal - ni@bbzpcagho12: -" with a menu bar (File, Edit, View, Terminal, Tabs, Help). It shows instructions for activating and deactivating a conda environment. The user runs `$ conda activate envlynx`, and the prompt changes from `(base)` to `envlynx`.

```
# To activate this environment, use
#
#     $ conda activate envlynx
#
# To deactivate an active environment, use
#
#     $ conda deactivate

$ conda activate envlynx

(envlynx) ~
```

on Windows 10 using Anaconda Prompt

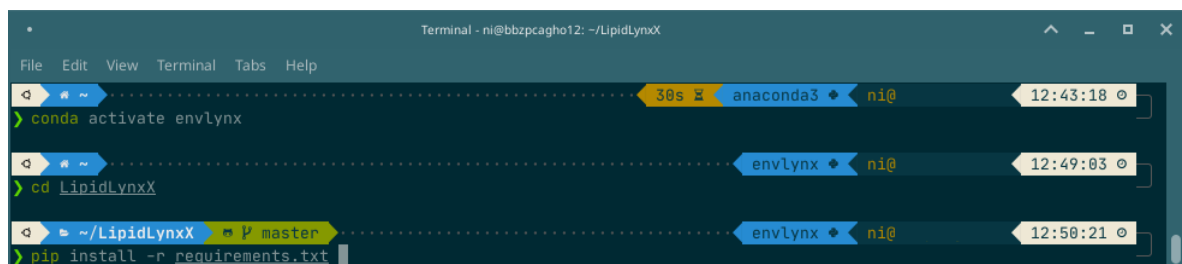
An Anaconda Prompt window showing the command `(base) C:\WINDOWS\System32>conda activate envlynx` and the resulting prompt `(envlynx) C:\WINDOWS\System32>`.

```
(base) C:\WINDOWS\System32>conda activate envlynx
(envlynx) C:\WINDOWS\System32>
```

Now you can navigate to LipidLynxX source code folder and install required packages using file `requirements.txt`.

```
cd LipidLynxX
pip install -r requirements.txt
```

You might have to type `y` for `enter` to confirm the installation of a list of packages.

A terminal window showing the user navigating to the `LipidLynxX` directory and installing packages from `requirements.txt`. The prompt changes from `(base)` to `envlynx` and then to `~/LipidLynxX`.

```
conda activate envlynx

(envlynx) ~
$ cd LipidLynxX
(envlynx) ~/LipidLynxX
$ pip install -r requirements.txt
```

Wait until you see the notification message that a list of packages has been successfully installed.

A terminal window showing the output of `pip install -r requirements.txt`. It lists the packages being installed and their versions, followed by a confirmation message.

```
Building wheel for future (setup.py) ... done
Created wheel for future: filename=future-0.18.2-py3-none-any.whl size=491058 sha256=e67f97a479d28c83f9d342e56cd99ab06458bdda6af94f11fb4ca084e4c72913
Stored in directory: /home/ni/.cache/pip/wheels/56/b0/fe/4410d17b32f1f0c3cf54cdfb2bc04d7b4b8f4ae377e2229ba0
Successfully built Flask-Compress Flask-Script openpyxl pyrsistent et-xmlfile future
Installing collected packages: Cython, itsdangerous, MarkupSafe, Jinja2, Werkzeug, click, Flask, Flask-Compress, six, pytz, aniso8601, Flask-RESTful, Flask-Script, WTForms, Flask-WTF, zipp, importlib-metadata, attrs, pyrsistent, jsonschema, lxml, pyparsing, numpy, cyclo, Kiwisolver, python-dateutil, matplotlib, natsort, jdcal, et-xmlfile, openpyxl, packaging, pandas, pluggy, wcwidth, more-itertools, py, pytest, coverage, pytest-cov, regex, idna, chardet, urllib3, requests, requests-file, xlrd, xlwt, pyzmq, greenlet, gevent, future, msgpack, zerorpc

Successfully installed Cython-0.29.13 Flask-1.1.1 Flask-Compress-1.4.0 Flask-RESTful-0.3.7 Flask-Script-2.0.6 Flask-WTF-0.14.3 Jinja2-2.11.2 MarkupSafe-1.1.1 WTForms-2.2.1 Werkzeug-1.0.0 aniso8601-8.0.0 attrs-19.3.0 chardet-3.0.4 click-7.1.1 coverage-5.1 cyclo-0.10.0 et-xmlfile-1.0.1 future-0.18.2 gevent-1.5.0 greenlet-0.4.15 idna-2.9 importlib-metadata-1.6.0 itsdangerous-1.1.0 jdcal-1.4.1 jsonschema-3.2.0 Kiwisolver-1.2.0 lxml-4.4.2 matplotlib-3.1.1 more-itertools-8.2.0 msgpack-1.0.0 natsort-7.0.1 numpy-1.18.1 openpyxl-3.0.3 packaging-20.1 pandas-1.0.3 pluggy-0.13.1 py-1.8.1 pyparsing-2.4.7 pyrsistent-0.16.0 pytest-5.4.1 pytest-cov-2.7.1 python-dateutil-2.8.1 pytz-2019.3 pyzmq-19.0.0 regex-2020.2.20 requests-2.23.0 requests-file-1.4.3 six-1.14.0 urllib3-1.25.8 wcwidth-0.1.9 xlrd-1.2.0 xlwt-1.3.0 zerorpc-0.6.3 zipp-3.1.0

(envlynx) ~/LipidLynxX
```

Then you can start LipidLynxX using following command:

```
python LipidLynxX.py
```

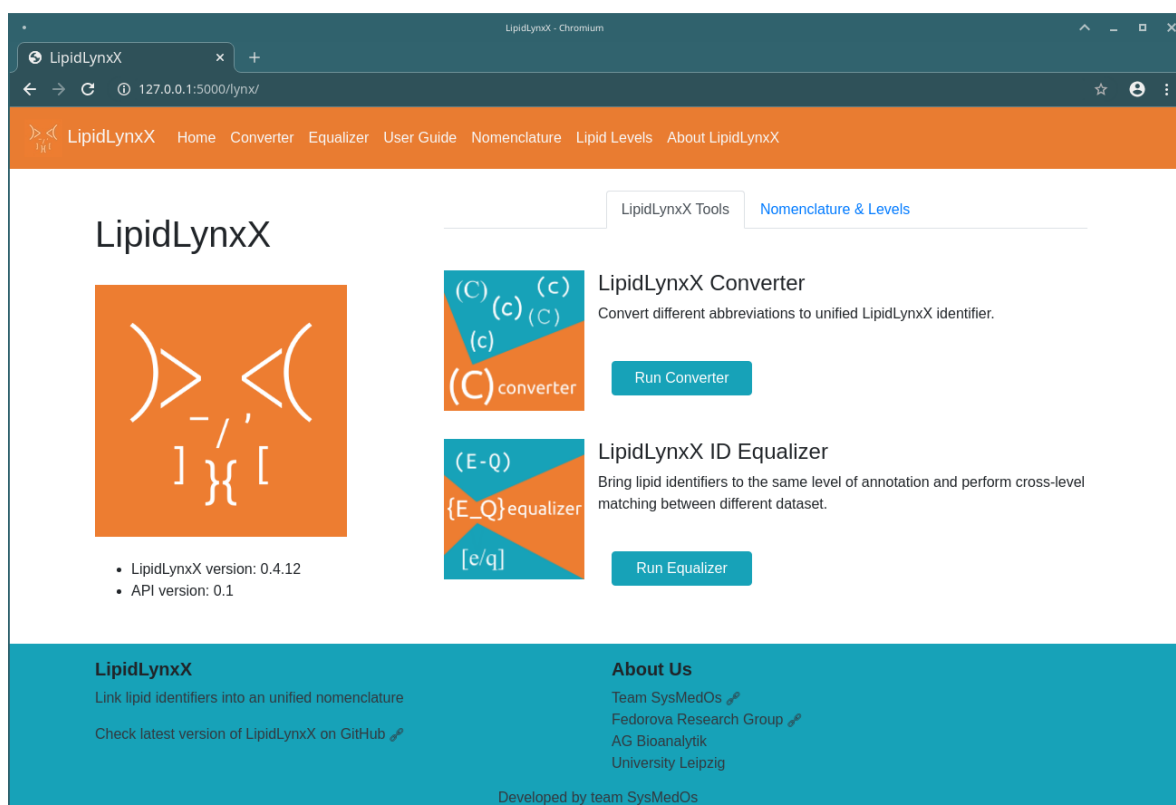
```
Terminal - ni@bbzpcagho12: ~/LipidLynxX
File Edit View Terminal Tabs Help
~ /LipidLynxX master envLynx n1@ 12:53:55
python LipidLynxX.py
```

After some debug information, you will see following information:

```
Terminal - python LipidLynxX.py
File Edit View Terminal Tabs Help
127.0.0.1 - - [16/Apr/2020 12:56:28] "GET /lynx/ HTTP/1.1" 200 -
127.0.0.1 - - [16/Apr/2020 12:56:28] "GET /lynx/ HTTP/1.1" 200 -
127.0.0.1 - - [16/Apr/2020 12:56:29] "GET /static/images/LipidLynxX_Logo_banner.jpg HTTP/1.1" 200 -
127.0.0.1 - - [16/Apr/2020 12:56:29] "GET /static/images/LipidLynxX_Logo.png HTTP/1.1" 200 -
127.0.0.1 - - [16/Apr/2020 12:56:29] "GET /static/images/converter_logo.png HTTP/1.1" 200 -
127.0.0.1 - - [16/Apr/2020 12:56:29] "GET /static/images/equalizer_logo.png HTTP/1.1" 200 -
127.0.0.1 - - [16/Apr/2020 12:56:29] "GET /static/images/nomenclature_logo.png HTTP/1.1" 200 -
```

And a browser window will pop up with LipidLynxX interface using link:

<http://127.0.0.1:5000/lynx/>



## Step by step tutorial

LipidLynxX currently have two major modules:

- LipidLynxX Converter
  - Convert different annotations to uniform LipidLynxX ID
- LipidLynxX Equalizer
  - Bring lipid identifiers to the same level of annotation and perform cross-level matching between different dataset

### Test files:

- Test input file: `doc/sample_data/input`
- Test output example files: `doc/sample_data/output`

## How to use LipidLynxX Converter


For Conversion, type/paste your lipid annotations or choose your .xlsx or .csv files. Press “convert abbreviations” or “convert table”, wait for results. You will see the output on the right-hand side or just download the table with converted IDs.

## Convert by text input

- Paste list of abbreviations in the text input field and press “convert abbreviations”.

- You can find example input in file

`doc/sample_data/input/LipidLynxX_conveter_test.txt`

 **LipidLynxX**

[Home](#) [Converter](#) [Equalizer](#) [User Guide](#) [Nomenclature](#) [Lipid Levels](#) [About LipidLynxX](#)

## LipidLynxX Nomenclature Converter

### Input lipid abbreviations

Paste lipid abbreviations below:

palmitic acid  
DHA  
HETE  
DPPE  
PlasmanyI-PC O-16:0\_18:2  
GPEtn(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))  
Cer(t18:0/26:0)  
SM(d18:1/26:0)  
MG(16:0)  
DG(16:0/18:2(9Z,12Z)/0:0)[iso2]  
TG(16:0/18:0/18:2(9Z,12Z))[iso6]  
TG(16:0/18:2/HETE)

Convert abbreviations



### Upload table

Choose File No file chosen

Support .csv or .xlsx format

Convert table

**LipidLynxX**  
Link lipid identifiers into an unified nomenclature

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Team SysMedOs   
Fedorova Research Group   
AG Bioanalytik  
University Leipzig

Developed by team SysMedOs

- You will see the output on the right-hand side or just download the table with converted IDs.

- You can find example output `doc/sample_data/output/LipidLynxX-converter_from_text.xlsx`



# LipidLynxX Nomenclature Converter

## Input lipid abbreviations

Paste lipid abbreviations below:

```
palmitic acid
DHA
HETE
DPPE
Plasmanyl-PC O-16:0_18:2
GPEtn(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
Cer(t18:0/26:0)
SM(d18:1/26:0)
MG(16:0)
DG(16:0/18:2(9Z,12Z)/0:0)[iso2]
TG(16:0/18:0/18:2(9Z,12Z))[iso6]
TG(16:0/18:2/HETE)
```

Convert abbreviations

## Upload table

Choose File No file chosen

Support .csv or .xlsx format

Convert table

## LipidLynxX output

Save output as .xlsx file



### Converted abbreviations

```
palmitic acid -> FA16:0
DHA -> FA22:6<{4Z,7Z,10Z,13Z,16Z,19Z}>
HETE -> FA20:4<OH>
DPPE -> PE(16:0/16:0)
Plasmanyl-PC O-16:0_18:2 -> PC(O-16:0_18:2)
GPEtn(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) ->
PE(18:0/22:6<{4Z,7Z,10Z,13Z,16Z,19Z}>)
Cer(t18:0/26:0) -> Cer(18:0/3/26:0)
SM(d18:1/26:0) -> SM(18:1/2/26:0)
MG(16:0) -> MG(16:0)
DG(16:0/18:2(9Z,12Z)/0:0)[iso2] ->
DG(16:0/18:2<{9Z,12Z}>/0:0)
TG(16:0/18:0/18:2(9Z,12Z))[iso6] ->
TG(16:0/18:0/18:2<{9Z,12Z}>)
TG(16:0/18:2/HETE) -> TG(16:0/18:2/20:4<OH>)
```

### LipidLynxX

Link lipid identifiers into a unified nomenclature

### About Us

Team SysMedOs   
 Fedorova Research Group   
 AG Bioanalytik  
 University Leipzig

Developed by team SysMedOs

## Convert by table input

- Press "Choose file"

# LipidLynxX Nomenclature Converter

## Input lipid abbreviations

Paste lipid abbreviations below:

Convert abbreviations

## Upload table

Choose File LipidLynxX\_test.xlsx



Support .csv or .xlsx format

Convert table

### LipidLynxX

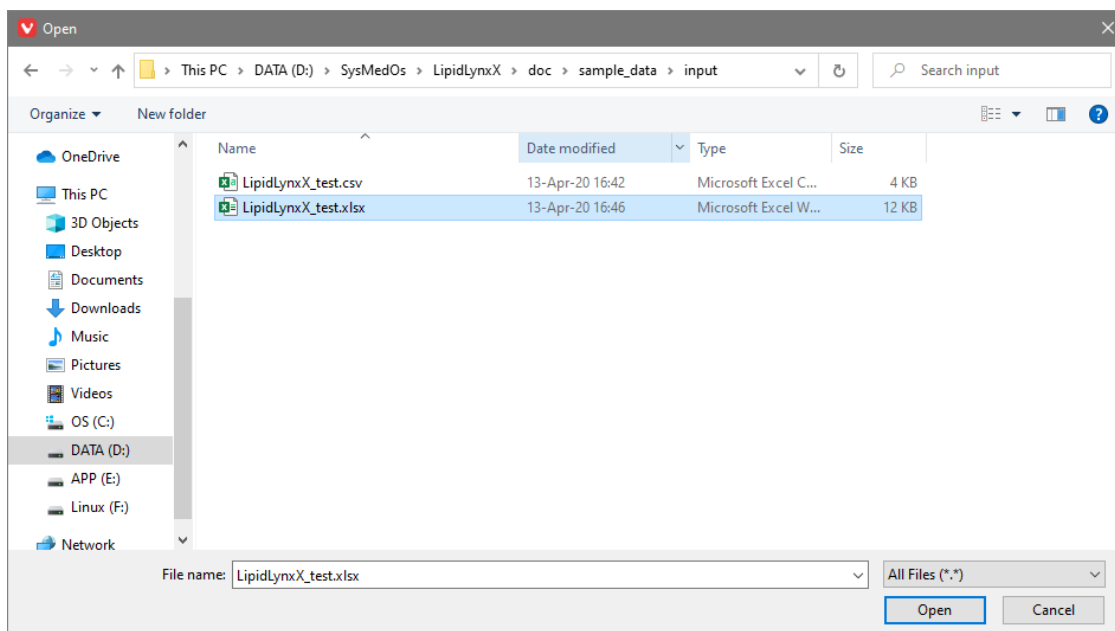
Link lipid identifiers into a unified nomenclature

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 Fedorova Research Group   
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 University Leipzig

Developed by team SysMedOs

- Select the input file in .xlsx or .csv format and press “Convert table”
  - You can use example file `doc/sample_data/input/LipidLynxX_test.xlsx`



- You will see the output on the right-hand side or just download the table with converted IDs.
  - You can find example output `doc/sample_data/output/LipidLynxX-Converter_from_table.xlsx`

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[Lipid Levels](#)
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## LipidLynxX Nomenclature Converter

### Input lipid abbreviations

Paste lipid abbreviations below:

[Convert abbreviations](#)

### Upload table

[Choose File](#) No file chosen

Support .csv or .xlsx format

[Convert table](#)

### LipidLynxX output

[Save output as .xlsx file](#)

### Converted abbreviations

```

FA14:0 -> FA14:0
PE(34:2) -> PE(34:2)
PE(O-34:2) -> PE(O-34:2)
PE(P-34:2) -> PE(P-34:2)
PIP(34:1) -> PIP(34:1)
PIP2(34:2) -> PIP2(34:2)
PIP3(34:2) -> PIP3(34:2)

```


## How to use LipidLynxX Equalizer

To Equalize, select LipidLynxX Equalizer tab from Home page. Select the level of annotations to which you would like to cross-match your lipid annotations (you can select more than one). For details on annotation levels see the tables on the right hand-side. Choose your datafile and press "Equalize". Download your results as .xlsx file.

### Convert by table input

- Press "Choose file" and select the input file in .xlsx or .csv format. Then select the level of annotations to which you would like to cross-match your lipid annotations (you can select more than one), in this case levels B0, D0 and D1 are chosen. Then you can press "Equalize" to start processing.

- o You can use example file `doc/sample_data/input/LipidLynxX_test.xlsx`


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## LipidLynxX ID Equalizer

LipidLynx ID Level Matrix

Unmodified Lipids

Modified Lipids

All Levels

Main levels for modified lipids

Bulk (B)	Discrete (D)	sn-Specific (S)
B0 PE(36:4)	D0 PE(16:0_20:4)	S0 PE(16:0/20:4)
	D0.1 PE(16:0_20:4<{5,9,12,15}>)	S0.1 PE(16:0/20:4<{5,9,12,15}>)
	D0.2 PE(16:0_20:4<{5Z,9E,12E,15E}>)	S0.2 PE(16:0/20:4<{5Z,9E,12E,15E}>)
Modification mass shift		
B1 PE(36:4<+46>)	D1 PE(16:0_20:4<+46>)	S1 PE(16:0/20:4<+46>)
Modification elemental composition		
B2 PE(36:4<+30,-2H>)	D2 PE(16:0_20:4<+30,-2H>)	S2 PE(16:0/20:4<+30,-2H>)
Modification type		
B3 PE(36:4<+20H,oxo>)	D3 PE(16:0_20:4<+20H,oxo>)	S3 PE(16:0/20:4<+20H,oxo>)
Modification position		
	D4 PE(16:0_20:4<+20H(8,11),oxo(14)>)	S4 PE(16:0/20:4<+20H(8,11),oxo(14)>)
Modification stereochemistry		
	D5 PE(16:0_20:4<+20H(8R,11S),oxo(14)>)	S5 PE(16:0_20:4<+20H(8R,11S),oxo(14)>)

# 1 Upload table

Choose File `LipidLynxX_test.xlsx`

Support.csv or .xlsx format

# 2 Set the LipidLynxX level(s)

- You can set one level (e.g. B0) or multiple levels separated by "," (e.g. B0,D0,D1).

Input LipidLynx level(s) here:

B0,D0,D1

# 3 Run Equalizer

Equalize


\* Learn more about [the LipidLynx ID Level Matrix](#)

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- You will see the output when the processing is finished and you can download the file in .xlsx format.

- o You can find example output `doc/sample_data/output/LipidLynxX-Equalizer_from_table.xlsx`


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## LipidLynxX ID Equalizer

LipidLynx ID Level Matrix

Unmodified Lipids

Modified Lipids

All Levels

Main levels for modified lipids

Bulk (B)	Discrete (D)	sn-Specific (S)
B0 PE(36:4)	D0 PE(16:0_20:4)	S0 PE(16:0/20:4)
	D0.1 PE(16:0_20:4<{5,9,12,15}>)	S0.1 PE(16:0/20:4<{5,9,12,15}>)
	D0.2 PE(16:0_20:4<{5Z,9E,12E,15E}>)	S0.2 PE(16:0/20:4<{5Z,9E,12E,15E}>)
Modification mass shift		
B1 PE(36:4<+46>)	D1 PE(16:0_20:4<+46>)	S1 PE(16:0/20:4<+46>)
Modification elemental composition		
B2 PE(36:4<+30,-2H>)	D2 PE(16:0_20:4<+30,-2H>)	S2 PE(16:0/20:4<+30,-2H>)
Modification type		
B3 PE(36:4<+20H,oxo>)	D3 PE(16:0_20:4<+20H,oxo>)	S3 PE(16:0/20:4<+20H,oxo>)
Modification position		
	D4 PE(16:0_20:4<+20H(8,11),oxo(14)>)	S4 PE(16:0/20:4<+20H(8,11),oxo(14)>)
Modification stereochemistry		
	D5 PE(16:0_20:4<+20H(8R,11S),oxo(14)>)	S5 PE(16:0_20:4<+20H(8R,11S),oxo(14)>)

# 1 Upload table

Choose File `No file chosen`

Support.csv or .xlsx format

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B0,D0,D1

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Equalize

\* Learn more about [the LipidLynx ID Level Matrix](#)

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Output generated!

Output file: LipidLynxX-Equalizer\_2020-04-13\_17-53-04.xlsx

Save output as .xlsx file

## How run LipidLynxX using Terminal commands

- LipidLynxX Converter

```
python LynxConverter.py -i doc/sample_data/input/LipidLynxX_test.xlsx -o doc/sample_data/output/LipidLynxX_test_converter_out.xlsx
```

- **LipidLynxX Equalizer**

```
python LynxEqualizer.py -l "B0,D0,D1" -i  
doc/sample_data/input/LipidLynxX_test.csv -o  
doc/sample_data/output/LipidLynxX_test_equalizer_out.xlsx
```

## Errors/bugs

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In case you experienced any problems with running LipidLynxX, please report an issue in the [issue tracker](#) or contact us.