GROMACS is a widely used, open source software suite to perform molecular dynamics simulations. It is designed to work on Linux/Unix based systems and is available as fully command-line based software.

Linux installation:

In the simplest way of getting GROMACS ready on Linux based machines like Ubuntu, running few commands through terminal can get it up and running.

Windows installation:

Though windows inherently don't support GROMACS, since Windows 10 version, Microsoft has added a provision to install Linux (Ubuntu) terminal, which can be utilised to install GROMACS. In other versions of Windows, it is fairly complicated for a newbie in computers. These steps are for Windows 10. Running these steps require active internet connection.

1. In windows applications, search and open option called **Turn Windows features on or off**
2. At the bottom of the list, you'll find a feature named **Windows subsystem for Linux.** Make sure to click on the small square box on it's left to turn on the feature
3. Click ok and now open **windows store**
4. Search for an app called Ubuntu
5. Install it.

Once Ubuntu is installed, open that app from your windows and issue following commands one by one to install Gromacs.

1. sudo apt-get update
2. sudo apt-get upgrade
3. sudo apt-get install gcc
4. sudo apt-get install cmake
5. sudo apt-get install build-essential
6. sudo apt-get install libfftw3-dev
7. sudo apt-get install gromacs

https://www.youtube.com/watch?v=S6n5dRVMM7w&feature=youtu.be

This YouTube video explains and shows the steps properly in case any doubt. You can also reach out to me on WhatsApp if any issues.