User Guide

Version:	v0.1
Date:	July 2022
Target(s):	• Researchers from experimental groups • Internship 2022 Mentoring • FYP 2022-2023 (if necessary)

* For any issues or comments on this set of materials, please contact me via email at: lokwanng@life.hkbu.edu.hk

1. Before you start, please read the information in doc -> 0-README-AND-OUTLINE-XXX.pdf for a brief introduction and the outline of this set of material.

2. Check README.txt for some other instructions, particularly on the programs to be installed locally.

3. Suggested order of using the provided documents:

	Handout	Tutorial
1	(README.txt) 0-README-and-outline.pdf	/
2	1-minimal-biochem.docx	/
3	2-molstruc-3D.docx	/
4	3-free-compchem-resources.docx	demo0-install.pdf
5	4-quick-eval-ex1-and-limit.docx	demo1-manual-fit-eval.pdf

4. A more generic installation instruction for the user to install **ALL** the software at once can be found in doc -> tutorial -> demo0-install.pdf. See README.txt if you would like to use a certain program that is already installed on your computer.

5. If you **ONLY** want to try the simplified workflow of protein-ligand complex evaluation and have all the required programs working, you may directly proceed to check doc -> tutorial -> demo1-manual-fit-eval.pdf. Note that only partial support to non-Windows environments is available at this moment.