Codecheck peer review of [Replication of Partial Least Squares Discriminant Analysis on Metabolomics NMR/MS Data](#)

Do the generated outputs match the ones in the paper in the target group's repo?

Matthew, Anmol, Juan, and Andres attempted to download the required packages but all failed. Maggie was the only one that was able to download and replicate the figures but, yes, we were successfully able to recreate Figure 2, 3 and 4 from the experiment.

Are the differences relevant or not?

There are no differences between the figures produced by our replication to those from the other replication team. We are unsure as to what some of the figures are replicating from the original project.

Are used pieces of software and data properly CITED and with suitable LICENSES?

Yes, all pieces of software are cited and have suitable licenses. However, the primary required library for the project was very difficult to install, and not all members were able to do it on their platforms.

Are open formats (text-based) included?

Yes, the files are found on git and maintained by the original organization, the MetaboAnalyst group, for open access and use.

Is data and software FAIR?

The data is 'FAIR', but software is only 'FA'. Despite being able to find and download the required software, only one team member was able to successfully install all dependencies and reuse it, this member was the only one using macOS which could have an impact in the installation success. Additionally, we had path problems referencing data and image files within the code that we had to resolve.