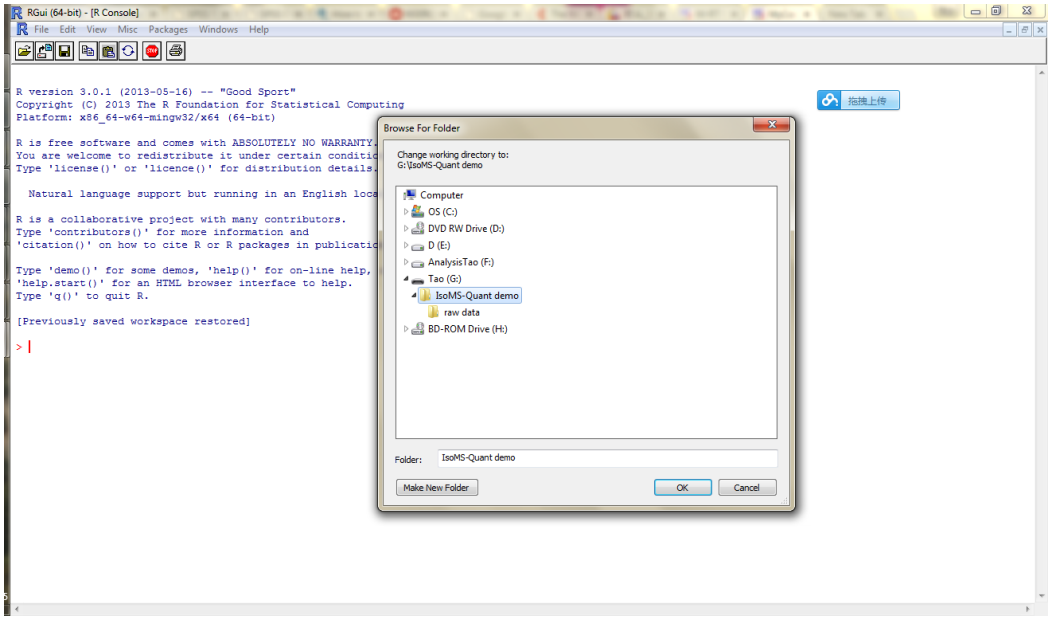
IsoMS-Quant User Manual (Version 1.0; Apr 15, 2015)

- IsoMS-Quant is a program written in R for recalculating the peak intensity ratio using the chromatographic peak area information. This program is part of the data processing software used for the chemical isotope labeling (CIL) LC-MS metabolomics platform.
- The IsoMS-Quant script is freely available for non-commercial use from www.mycompoundid.org.
- The instruction for using the IsoMS-Quant program is given below.

1) Download the IsoMS-Quant script from MyCompoundID.org.
2) Assign the folder of IsoMS-Quant as the working folder of RGui by clicking: File → Change dir… (see below).



3) Open the IsoMS-Quant script (see below) and change the parameters therein (see Table 1 for the explanation of these parameters).

```
########################################
# This is a script to do peak reconstruction after the zero-fill process
# Tao Huan, APril, 09, 2015
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########################################
# This is the setting part
file.path <- "G:/IsoMS-Quant demo/"
raw.file.path <- "G:/IsoMS-Quant demo/raw data/"
mz.tol = 5 # default 5 ppm
rt.tol = 30 # default 30 seconds
int.uplimit <- 1e7 # Saturation intensity threshold
########################################
```
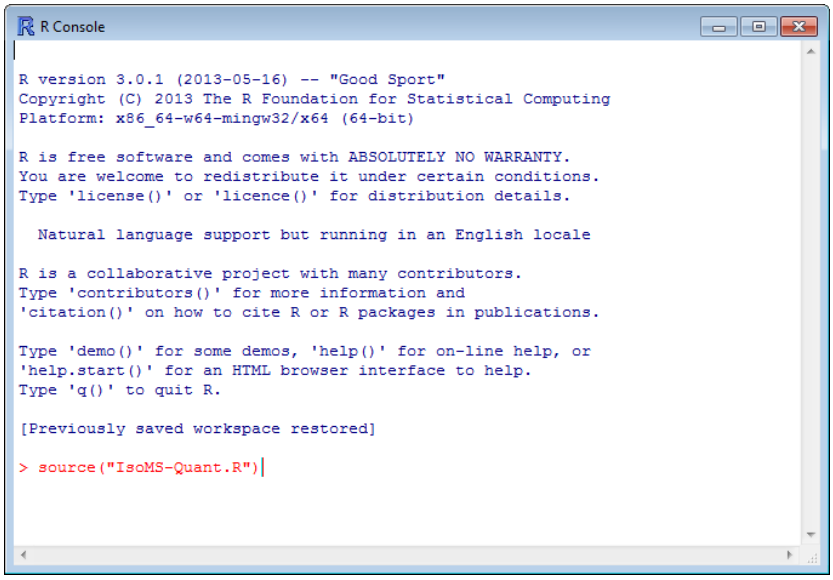

Table 1. IsoMS-Quant parameters that need to be changed according to the user's LC-MS instrumental conditions.

Parameter	Function
file.path	Set the data path to the folder that contains the zero-filled

	metabolite-intensity matrix
raw.file.path	Set the data path to the folder that contains all the raw LC-MS data containing all the peak information
mz.tol	Set the mz tolerance for the IsoMS-Quant processing
rt.tol	Set the retention time tolerance for the IsoMS-Quant processing
int.uplimit	Set the mass intensity saturation threshold

4) Save the parameter changes to the script. Type in the command code in RGui as shown in red in the following screen shot and press enter to run the script.



5) After running the script, a new csv file named "After_reconstruction_ratio.csv" will be created. This csv file contains the IsoMS-Quant result.