How to use the traceranalysis program

1. Organise your data such that the samples are in rows and isotopomers are in columns.

Eg like this:

**Table 1**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | 13C1 | 13C2 | 13C3 | 13C4 | 13C5 |
| No tracer 1 |  |  |  |  |  |
| No tracer 2 |  |  |  |  |  |
| No tracer 3 |  |  |  |  |  |
| Tracer 1 |  |  |  |  |  |
| Tracer 2 |  |  |  |  |  |
| Tracer 3 |  |  |  |  |  |

2. Determine the average values for no tracer samples in your data set.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | 13C1 | 13C2 | 13C3 | 13C4 | 13C5 |
| No tracer average |  |  |  |  |  |

Eg like this:

**Table 2**

1. Copy and paste ONLY THE VALUES (ie the part in blue) into a new excel file and save this as a .CSV file named according to the following scheme:

**‘{your sample name}\_averages.csv’**

**NOTE: If you are using excel to make .csv files there can be an error reading in this file if you have used extra cells that do not contain data at the point of saving. To fix this, right click and clear contents in empty cells next to your data.**

1. Copy and paste ONLY THE VALUES of your data set (ie the blue part in step 1) into a new excel file and save this as a .CSV file named according to the following scheme:

**‘{your sample name}\_data.csv’**

1. Repeat the above steps for all of your samples. Different samples will have different sample file names.
2. Transfer all the .csv files into the ‘test’ folder within the tracer\_analysis folder.
3. **Copy** ‘traceranalysis.py’ into the test folder and open in IDLE and run the program.
4. The results will appear as files labelled ‘{your sample name}\_output.csv’. The output is % representation of each isotopmer in each sample (to 1 decimal place) in the same order as in table 1.
5. Save your results and empty the test folder for next time.

Let me know if you have any problems or suggestions– s.trefely@gmail.com

Enjoy!