

# User manual

## TargetLynx (Waters, US) output files combination tool

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## 1. Abstract

The TargetLynx (Waters, US) software is a widely used tool for peak identification and compounds quantification of UPLC-TQ/MS instruments. Currently, the multiple output files (.txt) of this software cannot be applied directly for data analysis. Researchers have to spend a lot of time for format conversion and data combination.

A based software named “TQ combination” was developed by using C# in Visual Studio platform. The input of this soft are the .txt files provided by TargetLynx (1 file per sample) and the output is 4 .csv files with peak area, peak height, peak response and concentration respectively, of all the samples. The output files can be imported into universal data analysis softs such as SPSS, SIMCA, R, matlab, Graphpad and so on.

The GUI based software is green and doesn't need any installation.

## 2. Application

### 2.1 Set up the format of TargetLynx output files

In the TargetLynx result main window, click the white space, select “change column order” option (fig.1), adjust the order as Fig. 2.

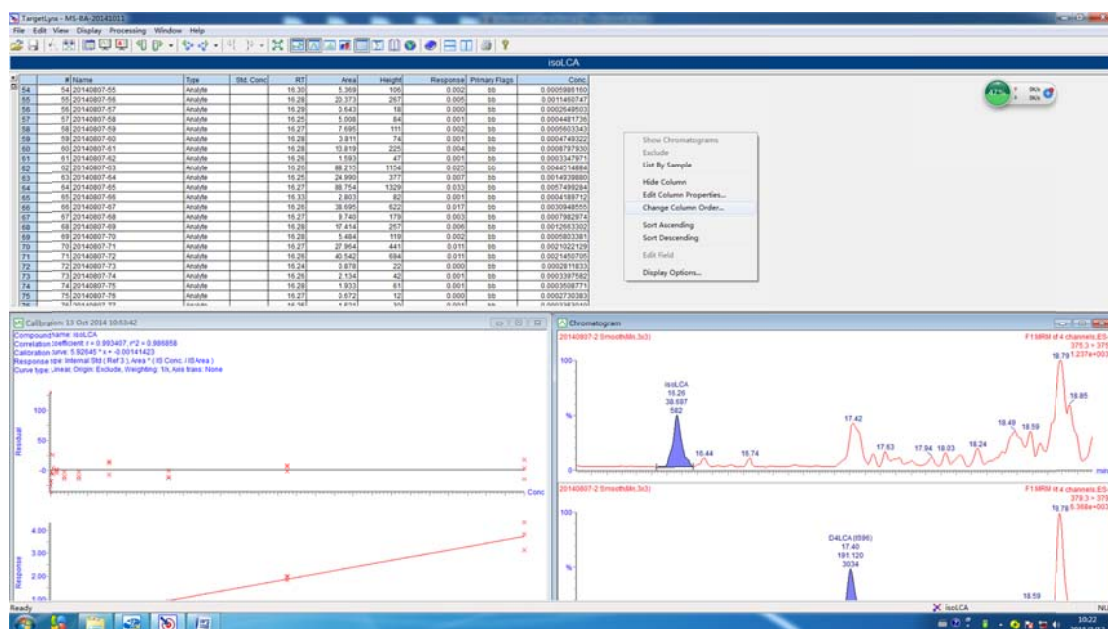


Fig. 1 Change column order.

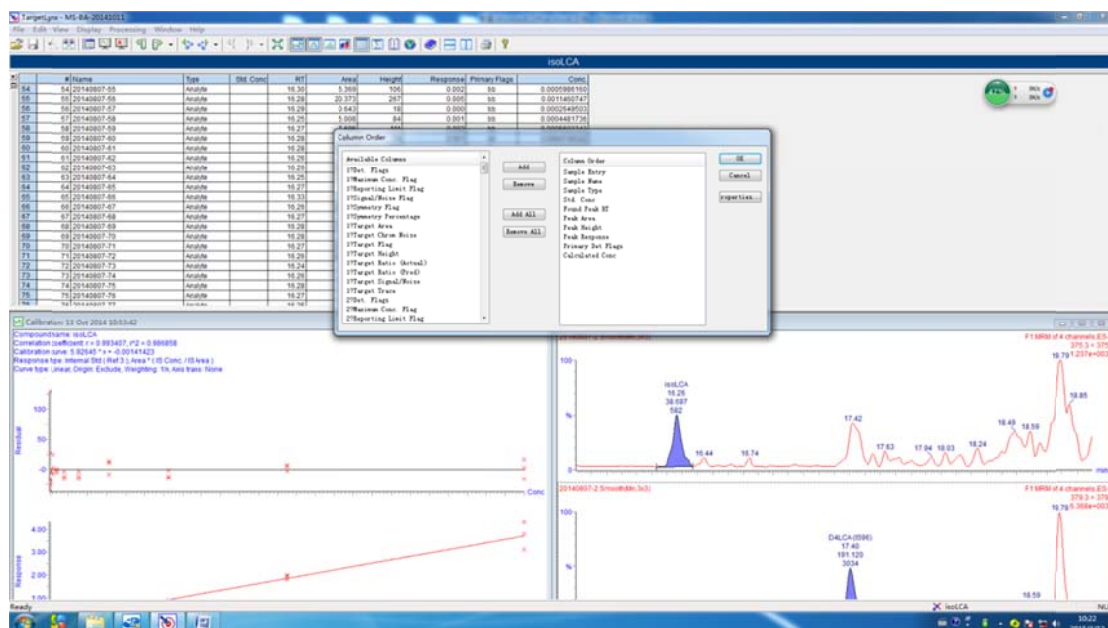


Fig. 2 set up the items and order of output files.

## 2.2 Export result files from TargetLynx

Select “file->export->Complete Summary” as Fig. 3 and export multiple .txt files to the target folder. You may export results of multiple batches separately. TQ combination is able to process and combine them together.

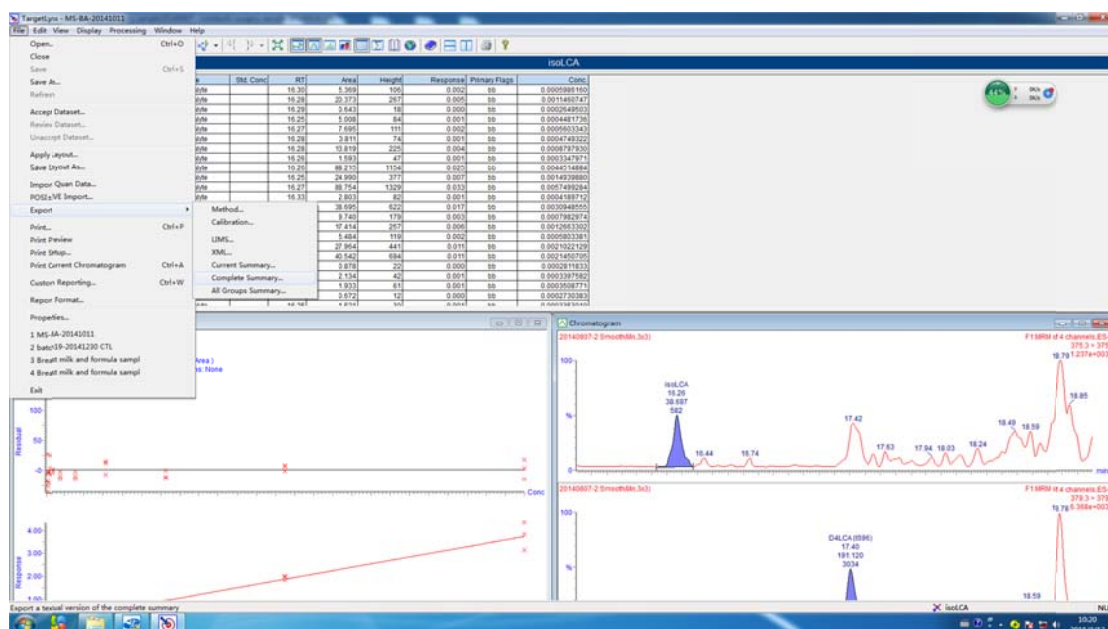


Fig. 3 Export multiple .txt results from TargetLynx-1.

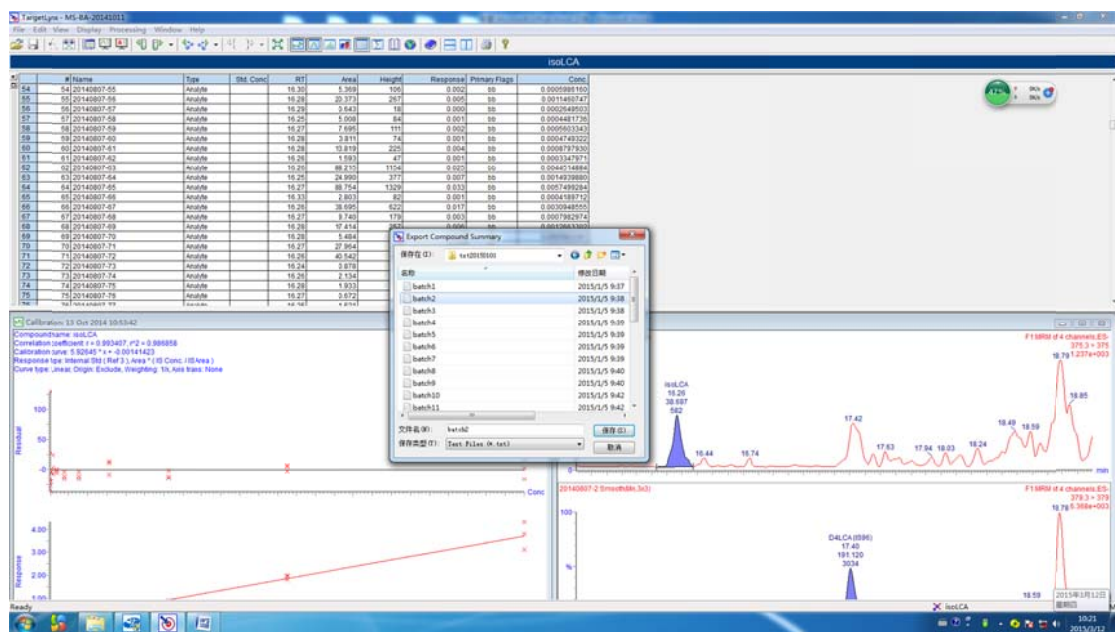


Fig. 4 Export multiple .txt results from TargetLynx-2.

## 2.3 Startup TQ combination

Click the exe file and start the software (Fig. 5). Installation is not required.

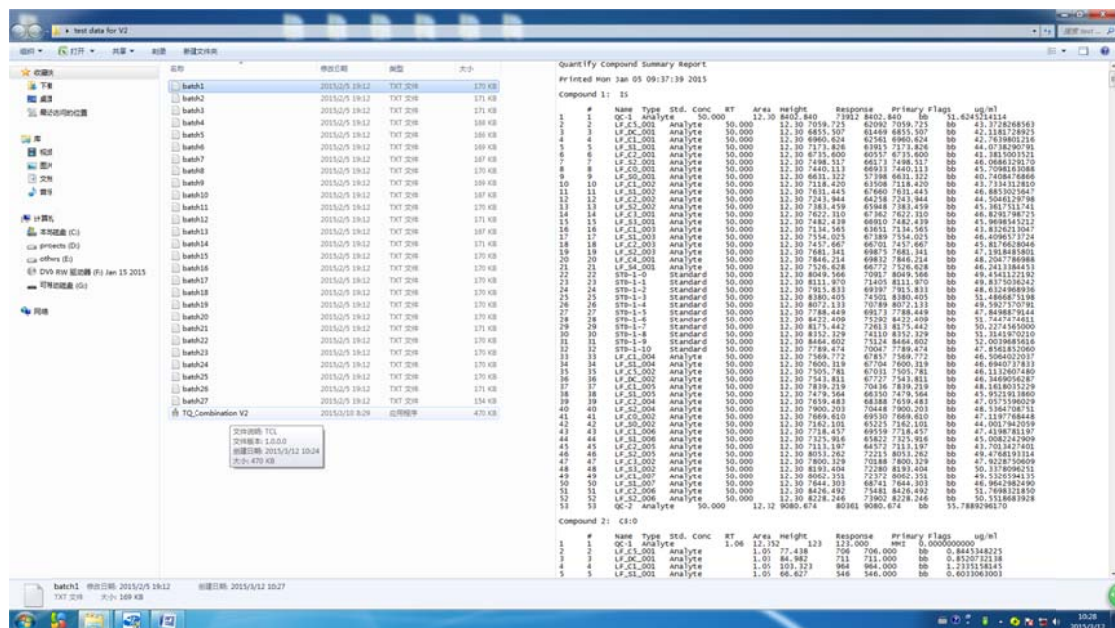


Fig. 5 startup the software.

## 2.4 Parameter setting

Click the “Select input” button and select the txt files awaiting for processing. Set the path and names of your output files. The default path and name are filled in as Fig. 6.

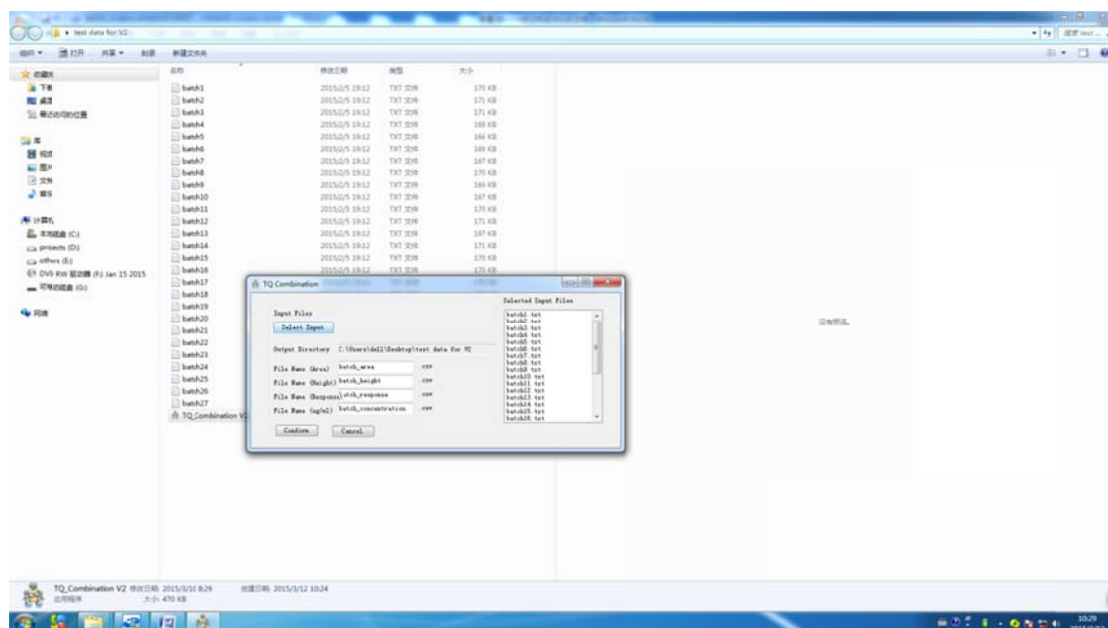


Fig. 6 parameter setting.

## 2.5 running

Click the “confirm” button and run the software. A success box will pop up after few seconds (Fig. 7).

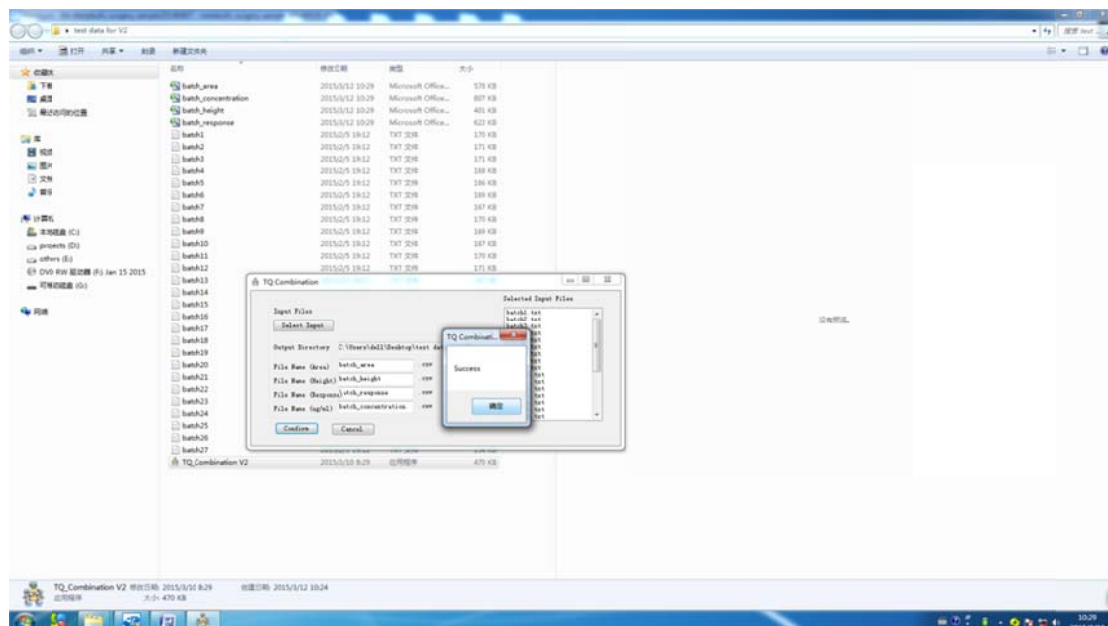


Fig. 7 running

## 2.6 The output files

Four .csv files (fig. 8), combined peak area, combined peak height, combined peak response and combined concentration, will be generated. Fig. 8 shows the format of the combined



concentration file. One sample per row and one compound per column. The first column is the txt file name and the second column is the sample name. Row 4-5 are the min and max RT of all the samples.

The screenshot shows a Microsoft Excel spreadsheet titled "batch\_concentration - Microsoft Excel". The spreadsheet contains a table with columns labeled A through Z. Column A is labeled "file name" and column B is labeled "sample name". Columns C through Z contain numerical data. The data is organized into rows for each sample, with the first two columns containing file and sample names, and subsequent columns containing numerical values for each compound. The data is organized into rows for each sample, with the first two columns containing file and sample names, and subsequent columns containing numerical values for each compound.

Fig. 8 Concentration file format.