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[Macedo* 6(2): February, 2019] ISSN 2349-4506
Impact Factor: 3.799

Global Journal of Engineering Science and Research Management

# CALLREG: AN APPLICATION FOR COLLECTION, TREATMENT AND MANAGEMENT OF MULTI-PURPOSE ANALYTICAL DATA

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**DOI: 10.5281/zenodo.2580281**

**KEYWORDS:** software; linearity; analytical chemistry; user-friendly.

## ABSTRACT

In this work, a new software for analytical data treatment was developed and tested. Results evidenced that there was no statistically significant difference between the data treated through the software herein developed and a standard data treatment software, what implies that out software may be a user-friendly tool to speed-up analytical data treatment.

## INTRODUCTION

Analytical data often requires strenuous and time-consuming treatment in order to provide relevant information to the analyst. In industries, such as pharmaceutical and chemical, Microsoft Office® package, *i.e.* excel, software is employed in this data treatment process. In order to provide routine dosage evaluations and linearity validations of chemical and pharmaceutical products, an analytical parameter (related to concentration) of the analyzed compound is plotted against its standard concentration, and then, linear regression is performed[1,2].

Linear regression is an extremely useful mathematical tool in chemical analysis, in the sense that it can numerically stipulate the relationship between two physical-chemical properties. Moreover, specter analysis often derive information from two mathematical properties, which are wave or peak amplitude and area under curve[3,4]. These parameters are usually obtained through the plotting of several graphs (*i.e.* 5 minimum points) in statistical software and manual evaluation of peak height or area under curve, followed by re-plotting of the curve points and performance of linear fitting analysis. Then, the calculated parameter of linear correlation (r) is used to validate the analytical procedure and the linear regression equation used to perform analyte dosing. This procedure although simple, is performed on daily basis within the chemical and pharmaceutical industry and, therefore, demands precious time of the analyst[5,6].

Since fast and reliable analysis are essential in the context of analytical procedures, simple tools capable of providing an user-friendly interface are highly regarded to speed-up data processing and allow more fluid operations. Henceforth, the aim of this work is to propose the development of an application intended for quick treatment of spectral data and also to manage linear regression parameters.

## MATERIALS AND METHODS

### Software Development and Evaluation

A CallReg application has been developed for Windows 64-bits. The software was written in MATLAB native language and developed in MATLAB App Designer UI. CallReg is available free in the following domain: https://isaacyvesl.wixsite.com/callreg. CallReg installer is available as a standalone application and includes MATLAB runtime libraries.

In overall, an algorithm for data collection within text (.txt) and excel (.xlsx) files determined by the user's selection, automatic retrieval of max amplitude/area under curve and storing of linear regression data was developed.

The main interface (Figure 1) includes: browsing buttons for file selection (maximum of 10 files), input boxes for concentration values, selection of file header checking, file type selection, amplitude and area under curve searches within selected files, visual panel of calibration curve plot and saving button for the writing of linear regression output (slope, intercept, calibration curve points and linear correlation value) in excel files.
Within the same interface the user may choose the analytical parameter to be automatically searched in selected files, see the calculation results and save the output linear regression parameters.

In order to compare mathematical calculations, Microsoft Office® Excel and Origin 8.0® software were used to perform the same linear regression as CallReg.

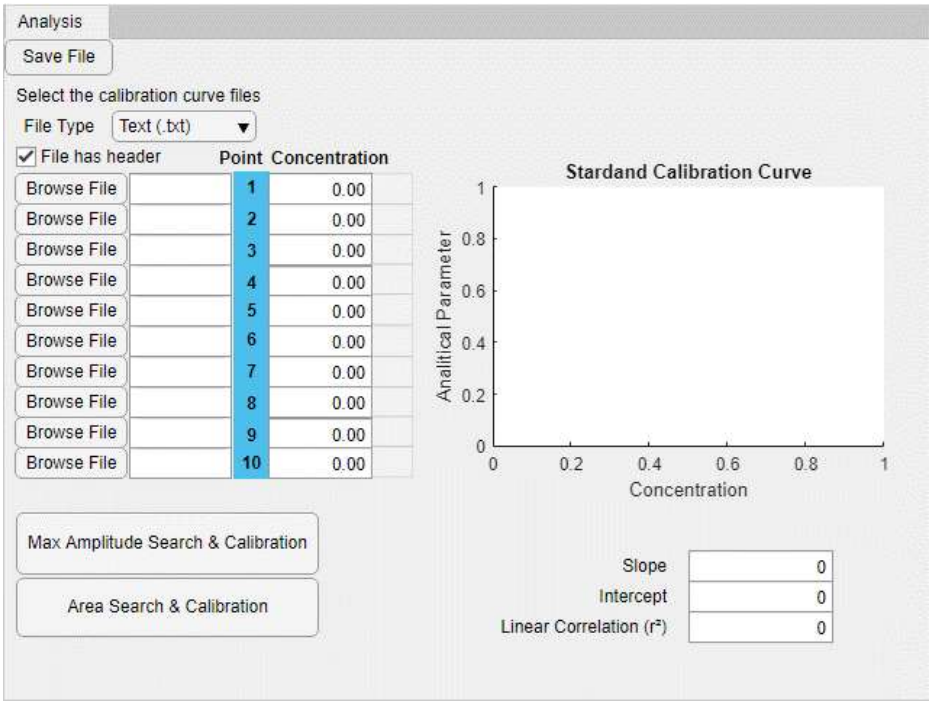


***Figure 1. CallReg main interface.***

## RESULTS AND DISCUSSION

### Determination of Omeprazole with Sample Specters

In order to evaluate the performance of CallReg, specters samples simulating chromatographic data of omeprazole were constructed. The specters peak amplitude and area under curve were made to be proportional to the concentrations of 10, 20, 30, 40 and 50 µmol.L$^{-1}$. The files were selected in CallReg. The corresponding concentrations were inserted into each box. The evaluation was made through area search (Figure 2A) and max amplitude search (Figure 2B). The resulting correlation equation found was $y = -4.226e^{-6} + 5.891e^{-7}x$ ($r = 0.989$) and $-2.234e^{-5} + 4.7696e^{-6}x$ ($r = 0.9798$) for area and amplitude, respectively. As expected, the linear regressions were different for the two different parameters and linearity was found in both cases.

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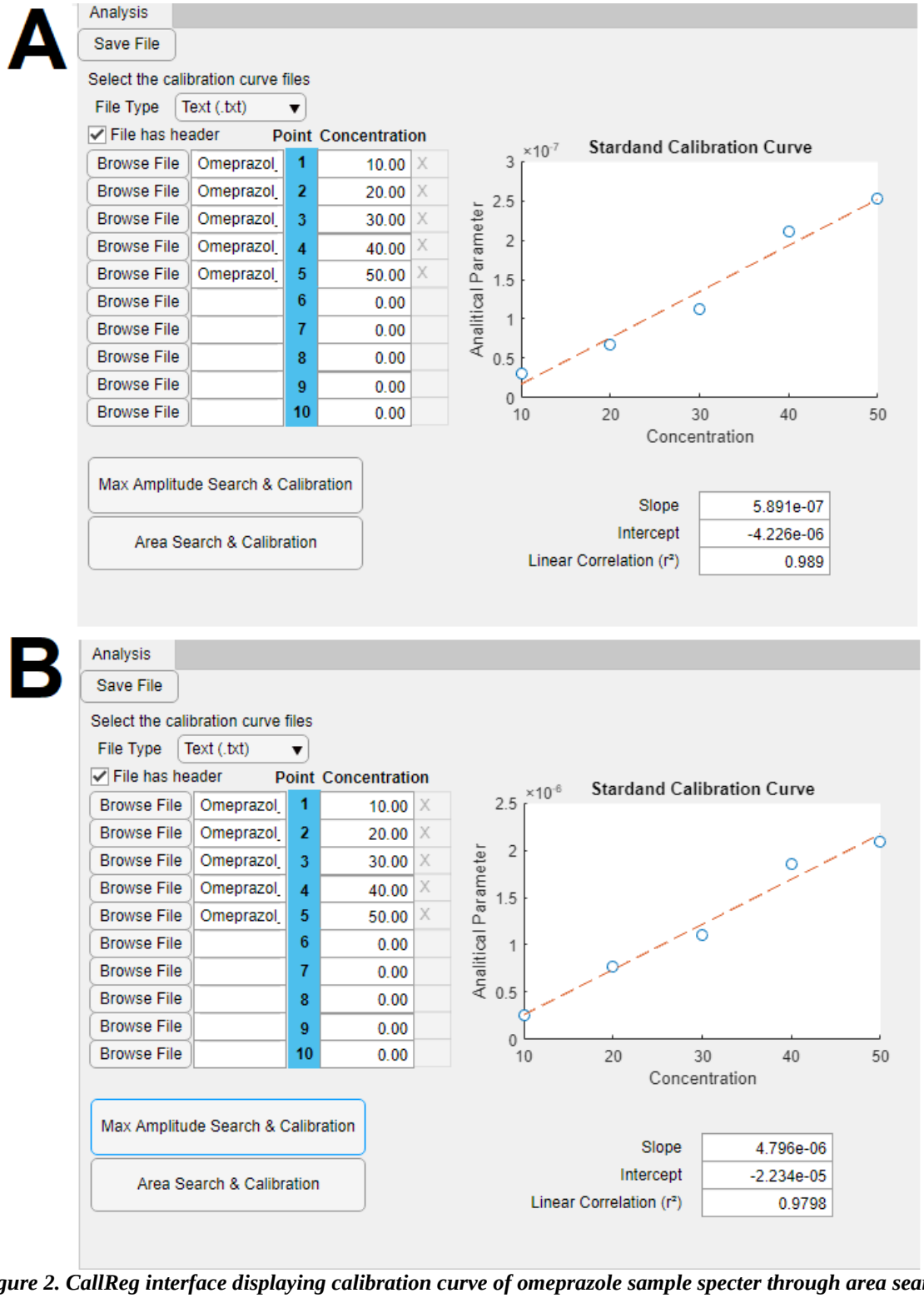


***Figure 2. CallReg interface displaying calibration curve of omeprazole sample specter through area search (A) and max amplitude search (B).***

**Comparison between data treatment software**

In order to ascertain the proposed CallReg application linear regression parameters, the same data treatment was performed in Microsoft Office® Excel (Figure 3A,B) and Origin 8.0® (Figure 3C,D).

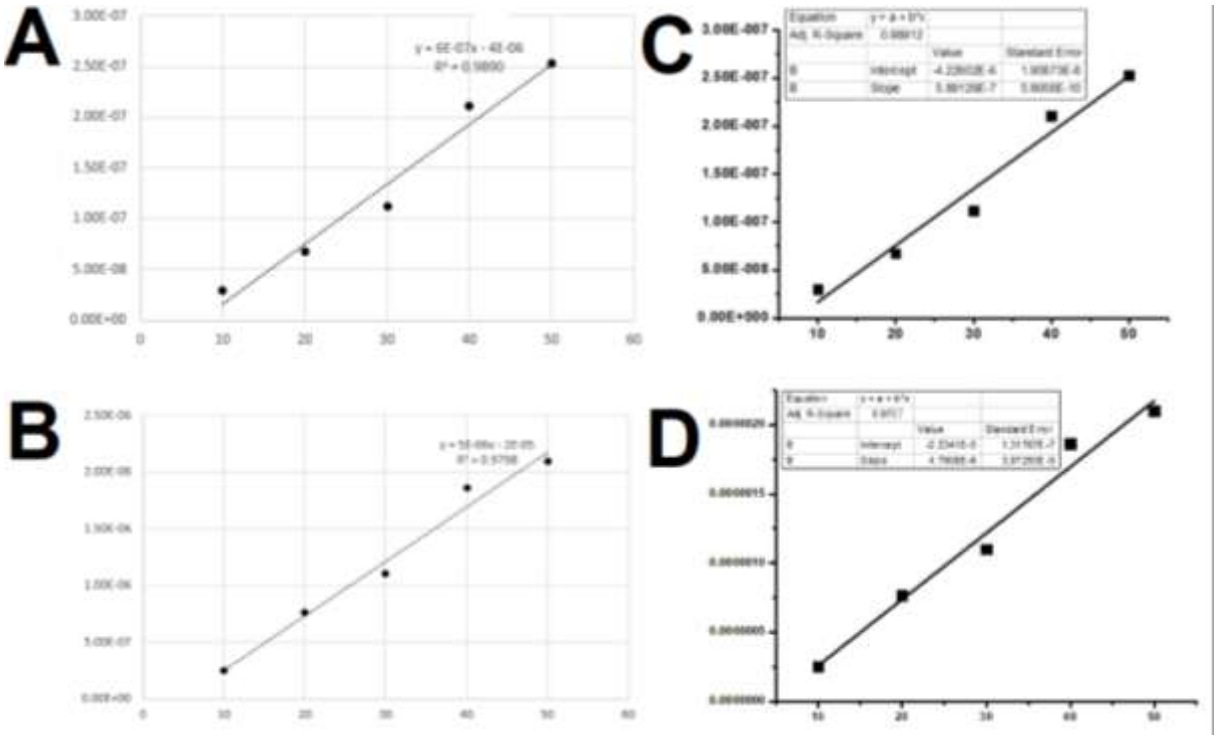


***Figure 3. Calibration curves of omeprazole sample specter with Excel® for area (A) and max amplitude search (B) and with Origin® for area (C) and max amplitude search (D).***

Excel® showed the same values for linear correlation of area (0.9890) and amplitude (0.9798), slope and intercept than those calculated through CallReg. However, it can be seen that Excel® linear regression display rounds slope and intercept values. Origin® linear correlation also displayed linear regression parameters virtually for area (0.98912) and amplitude (0.9797) virtually identical to CallReg. Origin® takes into account standard error and deviation in the linear regression and, thus, the values calculated slightly differ from CallReg and Excel®. However, these differences do not pose statistical significance.

## CONCLUSION

The proposed application was employed in the evaluation of calibration curves with specters from different analytical methodologies. This application can be used as a tool for the quick evaluation of specter files of calibration curves and storage of linear regression parameters.

The values calculated trough the proposed application show no relevant difference from the values calculated with popular used software. Thus, given the easiness of use, user-friendly interface and quick management of results, CallReg is a viable option to be used in data treatment.

Therefore, our group hopes that CallReg would be used as an auxiliary tool in industrial data management. We will develop an online browser application and standalone desktop application for Linux and Mac OS. Moreover, the data treatment algorithms herein demonstrated can be re-employed in add-ons to future software of more complex and wide functions.

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