Requirements 2D-GC visualization

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1 Introduction

2-dimensional Gas Chromatography (2D-GC) is a chemical technique to accurately identify and quantify small traces of compounds in samples. This analytical technique is used in Groningen to aid in the search for new biofuels. For this research, accurate and interactive software for 3D-visualization and analysis is necessary.

We aim to build a desktop app to visualise 2D-GC data, and try to work in comparative analysis, where the same analysis can be run smoothly on multiple samples.

2 MoSCoW

Critical Functional Requirements

- Show 2D-GC output .txt files as 3-dimensional graphs

- Show 2D-GC output .txt files as 2-dimensional graphs

- Integrate the matrix values between input x and y values, and label these peaks

Important Functional Requirements

- Be able to save the image with any attached user inputs such as integration or labels

- Input of extra integration parameters besides x and y (the client named only one example, we may need to ask what other parameters they need or want)

- Zooming, rotation, changing color of the visualization

- Peak selection (a basic way of implementation could be to have the user draw circles around a peak in a 2D visualization, and retrieve x and y from this)

- Be able to save peak data in a database, with any attached information, such as which sample it was from, integration value, labels etc.. The user should be able to retrieve previously saved information in a look-up table while looking at a new sample.

- Automatic peak finding

- Show 2D-GC output .txt files as 1-dimensional graphs (integrated data)

Useful Functional Requirements

- Pipelining for comparisons between samples

- Compound recognition/matching

- Signal to noise ratio convolution

Won't Do

- Web support

3 Meeting Log

Date	Meeting log
25/02/2019	Talked about and discussed the requirements document.

4   Change Log

Date	Author	Change log
15/02/2019	Oane Gros	Initial version
25/02/2019	All	Introduction and MoSCoW
04/03/2019	Wouter Brink, Oliver Strik	Added meeting and change logs
04/03/2019	Wouter Brink	Added title page