**Flanker: Computational Metabolomics**

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**Problem**

Metabolomics is the study of the entire set of metabolites in a biological system (Figure 1). It is an emerging and powerful technology that enables an unbiased and comprehensive view of system-wide metabolism.

![Computational Metabolomics Workflow](image)

**Market**

- **Current metabolomics market:** 2.38 billion, 2021 [2]
- **Comparison with past market:** 2.38 billion, 2016
- **Compound annual growth rate:** 14.6%

**Target group:** Researchers, industry workers, and students

**Market blank:** User-friendly, robust, yet comprehensive metabolomics data analysis tool

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**Existing Solutions**

<table>
<thead>
<tr>
<th>Solution</th>
<th>PROs</th>
<th>CONS</th>
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</thead>
<tbody>
<tr>
<td>XCMS</td>
<td>User-friendly online platform Multifunctional R package</td>
<td>Online version: ambiguous parameters R version: requires coding</td>
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<tr>
<td>MS-DIAL</td>
<td>Smooth workflow within data processing functionalities</td>
<td>Algorithm unable to modify No parameter optimization</td>
</tr>
<tr>
<td>XCMS</td>
<td>User-defined sub steps Result visualization</td>
<td>UI difficult to use Preliminary feature extraction</td>
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</tbody>
</table>

**Needs/Requirements/Specs**

- **User interface**
  - User friendly, intuitive, simplistic & modern
  - Application learning time
    - Quicker than existing solutions: ~ 1 hour
  - Metabolic data processing workflow
    - All-inclusive: feature extraction, evaluation & annotation
  - Automatic parameter optimization
  - Data visualization
    - Multiple types of plots for visualization
  - Integration with client provided code
    - R scripts for data processing
  - Sample processing time
    - < 20 min / file
  - Personalization setting
    - Customizable parameters and algorithms

**Our Solution – Flanker**

- C# based Windows 10 program developed in visual studio, based on UWP platform (Figure 2)
- Aesthetic & intuitive UI with light & dark themes
- Machine-learning based parameter optimization
- Integrates with client provided R scripts
- Allows users to upload custom algorithms
- 4 default plots for result visualization

**Competitive Distinction**

- More user friendly and faster to learn
- Option to customize or optimize parameters
- Comprehensive & robust: includes functionalities beyond all existing solutions

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**Test Summary**

Both user feedback and software tests were conducted to make sure Flanker satisfies requirements, the results are summarized below:

- UI user friendly rating (lab student feedback): 4/5
- User learning time: < 20 min
- User mis-clicks made using Flanker: < 6
- Integration with R code: able to execute various R scripts and retrieve results with < 2 sec delay
- Data processing time: < 5 min / file
- Max files processed simultaneously: 100
- Peak computer memory usage: ~70%

**Conclusion**

We conclude that Flanker is a comprehensive and robust bioinformatics software that meets all client requirements. Since Flanker contains all modules of metabolomics data analysis from feature detection to biological annotation, it can significantly increase research efficiency compared to previous solutions that only offer limited functionalities. Flanker’s user-friendly and intuitive interface would also make it possible for students and researchers without computational knowledge to produce meaningful results from bioinformatics analysis. Finally, Flanker’s versatility allows easy integration of additional algorithms which can expand its usage beyond metabolomics into the field of proteomics and lipidomics in the near future.

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**Reference / Bibliography**


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