'Free your data‘
Concepts of direct data transfers

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STOFF-IDENT data with only water relevant substances as first filter.

Using filtered data with other databases and tools to develop a score and improve results.

Browser / Web Application

Search via Excel files with mass targets

Search via Excel files with mass targets, fragment masses and retention time (using RTI)

Software of analytical hardware vendors

Single search

Search via Excel files with mass targets

Search via Excel files with mass targets, fragment masses and retention time (using RTI)

Further externals

Looking for and evaluating further tools and databases

Fragment masses and transformation products

In silico fragmentation

Mass spectral Database

eawag pps
Pathway prediction system (transformation product prediction)
Concepts

• Aim: Enable simple data import into a web-application without using a temporary export e.g. Excel
• Scenario: Open a web browser and transfer data into a web-application
• Unidirectional communication between a desktop and web-application
  – Using HTTP GET (1)
  – Using HTTP POST (2)

• Bidirectional communication between desktop and web-application (3)

• Three selected concepts - more valid approaches possible...
(1) Using HTTP GET


- Software of analytical hardware vendors
- Generate Link with data
- Open Browser on local Operating System
- Use Link in Browser
- Web Application with imported data

- Length of the URL restricted by browser
  - e.g. IE 1000 characters
- Not enough for the expected data
- Conclusion
  - Simple implementation
  - Not suitable for our requirements
(2) Using HTTP POST

- Advantages POST
  - No data limitation
  - Text and binary data

- Problem:
  - Open browser and send POST request
  - Not possible like using GET
  - No support from the browsers
  - Session handling limits the possibilities

http://www.for-ident.org/?mass=435.5188&formula=C24H29N5O3&...
(2) Using HTTP POST - the detour

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Read template html file
(2) Using HTTP POST – Template HTML

```html
<!DOCTYPE html>
<html>
  <head>
    <script src="execute.js"></script>
  </head>
  <body onload="post('http://www.for-ident.org/',
       {__data__});">
    </body>
</html>
```
(2) Using HTTP POST - the detour

- Software of analytical hardware vendors
- Read template html file
- Fill template with data (text or binary)
- Save temporary local html file
(2) Using HTTP POST – Executing HTML

```html
<!DOCTYPE html>
<html>
  <head>
    <script src="execute.js"></script>
  </head>
  <body onload="post('http://www.for-ident.org/',
               {mass: '435.5188', formula: 'C24H29N5O3', ...});">
  </body>
</html>
```
(2) Using HTTP POST - the detour

- Open Browser with temporary local html file
- Read template html file
- Fill template with data (text or binary)
- Save temporary local html file
- Software of analytical hardware vendors

- Browser executes embedded JavaScript (onLoad)
- Sending data via POST to Web-Application
- Web-Application prompts for user credentials
- User logs in
- Imported data is ready for processing
- Imported data is ready for processing

Imported data is ready for processing
(2) Using HTTP POST – Conclusion

- No data limit - suitable for our requirements
- Not limited to FOR-IDENT
- Data requirements can be defined in a template
- Read file and manipulate easily implemented
- But more effort than GET (1)
- JavaScript necessary
(3) Bidirectional communication – Import data

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Send data to Web Application

Receive ID

Create link with ID as GET parameter

Open Browser with link

Receive and store data

Generate and send ID

Web-Application prompts for user credentials

User logs in

Imported data is ready for processing

Data flow:
- Data from software of analytical hardware vendors is sent to the Web Application.
- The Web Application receives an ID and prompts the user for credentials.
- Once the user logs in, the imported data is ready for processing.
(3) Bidirectional communication – Export data

User requests results import

Handle results data

User process data

User mark results as ready

Web-Application receives ID

Web-Application sends results data

ID

results
(3) Bidirectional communication – Conclusion

• No data limit - suitable for our requirements

• Not limited to FOR-IDENT

• Bidirectional communication – Results flow directly back

• Technically complex

• Many technical possibilities of communication - complex and error-prone

• High costs in the implementation on both sides
Summary

• (1) GET
  – Minimal effort
  – Severely limited due to the small amounts of data
  – Unidirectional communication

• (2) POST
  – Defensible expense (file manipulation and program start)
  – Flexible (easily adaptable to other Web applications)
  – Dataset is not a limiting factor
    – Unidirectional communication

• (3) Bidirectional Communication
  – Biggest effort
  – Greatest benefit for users
  – High complexity => many pitfalls => many sources of error
Conclusion

Recommendation

(2) POST

Pragmatic approach
"Quickly" realized
Established technologies
Little Unknown
Thank you for your attention