Touching the core of reagents inventory management

Use of KNIME to Automate Data Transfer from Sharepoint to PerkinElmer

How Knime made unhappy-people happy and helped saving time

Fabio Rancati
Summary

- Background
  - Reagent’s workflow
  - Who was unhappy
  - Why

- What can be improved
- What can be automated

- Implemented workflows

- Who is happy now?
Background: the workflow

Purchase request done by Scientist

Annual declaration on purchased substances included in list of controlled

Reagents’ management workflow

SDS retrieval and company’s dB update

Upon delivery reagent’s info must be inserted into dB, labels printed and container placed into stockroom

https://www.opcw.org/
Background: the workflow

Copy&Paste was the highest level of automation.... When used Most important info of a reagent is its structure... conversion from SMILE or compound name
# Background

<table>
<thead>
<tr>
<th>Who was unhappy?</th>
<th>Why?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scientist</td>
<td>Error in reagents</td>
</tr>
<tr>
<td>Warehouse manager</td>
<td>Manual work Copy &amp; paste based</td>
</tr>
<tr>
<td></td>
<td>Data integrity</td>
</tr>
<tr>
<td></td>
<td>Frequent of errors</td>
</tr>
<tr>
<td></td>
<td>Time waste</td>
</tr>
<tr>
<td></td>
<td>Time consuming check for reagents</td>
</tr>
<tr>
<td></td>
<td>included in Controlled Substances list</td>
</tr>
</tbody>
</table>
So what?
Something can be improved

Request Form

Improve Purchase Request Form

Limit the possible sources of error
What can be automated

***AIM***
Eliminate any manual operation in workflow from the order to the reagents’ database for ~1000 reagents and ~2000 containers/year

**Perkin Elmer Inventory Enterprise**
Oracle based dB

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**Request Form**

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**SharePoint**

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**KNIME**
Open for Innovation

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Workflow implementation
Connection with MS SharePoint was not an easy task to complete.

Attempts done to use standard nodes was unsuccessful
Forum post was not helpful (Dec 2017)

At end we preferred to relay on a 3rd party commercial JDBC driver to be used in the classical database reader node
Site’s SSL certificate must be included in the cacerts dB in the JVM embedded in Knime

https://www.cdata.com/
Workflow Implementation: Check compound exists

Check if compound already exists:

Used the Perkin Elmer Oracle Cartridge function to recursively query Inventory for each compound SMILE and split dataset basing on the presence of a compound in the dB.

If compound exists it is excluded from registration.
Workflow implementation: retrieve density

For all new compounds call PubChem’s API to retrieve density when available using GET node. The obtained XML is parsed to extract value.
Workflow scheme: create dB record

Check if compound already exists

Register Compound data

Make use of Cartridge functions to convert SMILES into the proprietary format (BASE64_CDX) for the storing of molecule in the Oracle dB

Retrieve generated ID

CompoundID

Register Container data

Database hierarchy 1 compound to many containers

Open for Innovation

KNIME

CompoundID
Workflow scheme: create dB record

1. Check if compound already exists
2. Register Compound data
3. Register Container data

Database hierarchy: 1 compound to many containers
Workflow scheme: print labels

Text mining of ZPL file
Calculate expiry date
Loop BAT file execution to send TXT file to printer
Email report

Print Labels
Send email report
Workflow scheme: SDS and Risk phrases

If not received with the order, Reagent Management group retrieves SDS from the supplier site for those reagents included in the report received.

SDS PDF file are saved in Sharepoint db with metadata.
Workflow scheme: SDS and Risk phrases

If not received with the order, Reagent Management group retrieves SDS from the supplier site for those reagents included in the report received.

SDS PDF file are saved in Sharepoint db with metadata.
Background: the workflow

Annual declaration to the Italian Ministry on the use, import and export of controlled substances purchased
Do not forget any!

Crosscheck company’s reagents dB on 2 documents of Chemical Weapon precursor
Workflow scheme
Workflow implementation

Lists of controlled substances in digital format
Workflow implementation

Lists of controlled substances
In Digital format
## Workflow output

<table>
<thead>
<tr>
<th>QTY</th>
<th>UNIT</th>
<th>DATE</th>
<th>HANDLING PROCEDURES</th>
<th>SIMILARITY</th>
<th>REAGENT</th>
<th>PRECURSOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>g</td>
<td>28-Jun-19</td>
<td></td>
<td></td>
<td></td>
<td>![Chemical Structure 1]</td>
</tr>
</tbody>
</table>

- **M301**: Inativo per ingestione.
- **H534**: Sospettato di provocare alterazioni genetiche.

| 1,000 | g | 28-Jun-19 | | 0.9 | ![Chemical Structure 2] |

**Note:** The compounds are in digital format.
Who is happy now

<table>
<thead>
<tr>
<th>Who was unhappy?</th>
<th>Why is happy now</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scientist</td>
<td>No more error in reagents</td>
</tr>
</tbody>
</table>
| Warehouse manager | No manual work Copy&paste  
                           Data integrity guaranteed  
                           No errors in reagents structure  
                           60 min/week saved |

Check for reagents included in Controlled Substances lists done in few minutes  
No reagent excluded
Conclusion: Knime is the pivot of reagents’ management

Purchase request done by Scientist

Annual declaration on purchased substances included in list of controlled

SDS retrieval and company dB update

Upon delivery reagent’s info must be inserted into dB, labels printed and container placed into stockroom
Acknowledgment

Andrea Ciacci form S-IN Soluzioni informatiche - Workflow implementation

Roberto Forlani from Perkin Elmer – Support and for putting me in contact with

Andreas Muheim from Givaudan that gave me first suggestion on how use Knime with Inventory

The importance of the User Community!

Thank You!

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