Analytical Workflow and Knowledge Management

Waters AWM and ACD Software – an Useful Combination Implemented by an Interface

Bernd Undeutsch,
12th ACD/Labs European User Meeting.
ACD/SpecManager, ACD/Spectrum Database and ACD/C+H NMR Predictors and DB

Excellent Tools for

- Interpretation, assignment and reporting.
- Useable as spectroscopic knowledge database.
- Good prediction tool for the structure elucidation when based on a reliable data base.
Analytical Workflow Manager

Useful features

- Flexible Order Management
- „Invisible Work“ with AWM
- Interfaces
  - Chemical Lab Journal (developed by BayerBBS)
  - Configurable Instrument Agents
  - Long Time Archive System
  - Web Service API
"Quick Service“
only spectra generation, without validation of results
by analytical staff.
Chemist is responsible

Chemical Lab Journal with Ordering Tool

Waters AWM

NMR  MS  OPT

ACD SpecManager
Analytical Workflow within the Medicinal Chemistry

Chemical Lab Journal with Ordering Tool

Waters AWM

ACD SpecManager SpecDB

„Auftragsdienst“
Structure elucidation or confirmation.
Analytical staff orders the appropriate set of measurements.
Analyst is responsible.

NMR  MS  OPT

Orders
Analytical Workflow within the Medicinal Chemistry

Chemical Lab Journal with Ordering Tool

Waters AWM

ACD SpecManager SpecDB

Structure Elucidation

„Auftragsdienst“
Structure elucidation or confirmation. Analytical staff orders the appropriate set of measurements. Analyst is responsible.

NMR  MS  OPT

Spectra/Results

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NMR MS OPT

Spectra/Results
Necessary Functions and Properties of the Interface

All actions driven by ACD

- Automatic transfer from AWM to ACD Database and back
  - Import of all spectra within one order into one record, controlled by flags in AWM
  - Writing back of changed structures and result files (pdf)
Necessary Functions and Properties of the Interface

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- Automatic transfer from AWM to ACD Database and back
  - Import of all spectra within one order into one record, controlled by flags in AWM
  - Writing back of changed structures and result files (pdf)
- Report generation for the information transfer to the customer
  - Template driven
  - Easy to use
Necessary Functions and Properties of the Interface

All actions driven by ACD

• Automatic transfer from AWM to ACD Database and back
  - Import of all spectra within one order into one record, controlled by flags in AWM
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• Report generation for the information transfer to the customer
  - Template driven
  - Easy to use

• Automatic transfer of spectra and assignments
  - Corporate spectra database
  - Prediction database
Summary of Dataexchange between AWM and ACD
Summary of Data exchange between AWM and ACD

1. Order-Metadata
2. Structure
3. Spectra, -Metadata

report, PDF
Summary of Dataexchange between AWM and ACD

1. Order-Metadata
   - Structure
   - Spectra, -Metadata

2. Structure
   - report, PDF

3. Std-Nr
   - Elucidation text
Summary of Dataexchange between AWM and ACD

1. Order-Metadata
2. Structure
3. Spectra, -Metadata
4. Std-Nr
5. Elucidation text

Driven by ACD Automation Server

1H, 13C - Chemical Shifts and couplings

Interface driven
Using the interface interactively
Using the interface interactively

Start the analytical work!
Using the interface interactively

After selecting a report template and the spectra you can create a report and send it back to AWM, you can also transfer a changed structure.
Using the interface interactively

You get all new data after closing the order:
„Interpretation text“
„Std.-Nr.“
Using the interface interactively

Now you can set the status of a record from „work in progress“ to „to be published“
End of the Structure Elucidation Process
Start of the Knowledge Management

- Every member of the analytical staff has its own database
- Analyst decides when the structure elucidation process is finished
- The approval of data for the knowledge management process is done by setting the status „To be published“
Local „elucidation Databases“
PC-based

ACD Automationserver

ORACLE

AWM DB

API

Lo DB

Gr DB

BU DB

De DB

MW DB

HA DB

Be DB

Assignments Annotations
Shifts Couplings

ACD Enterprise Spektren DB

ACD Makro

ACD ¹H, ¹³C Prediction DB

„Export to Remote DB“

PC based
ACD Automation Server

- At night: transferring the assignments made during elucidation into the remote Database, making spectra and structures public.
- At night: transferring the assignments made during elucidation into the prediction Database, making the information public.
- At night: writing back the transfer status „Successful transfered“ or „Error during transfer“ into the elucidator databases.
- Taking control by:
  - Determining start- and stop-time of the AutomationServer
  - Inspecting several log-files
  - Receiving email in case of warnings
Next Steps

- Integration of NMR Workbook functionality into the elucidator databases (finished)
- Transfer of historical data from AWM into ACD enterprise database (ongoing)
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