

ELN-DIY-Meta

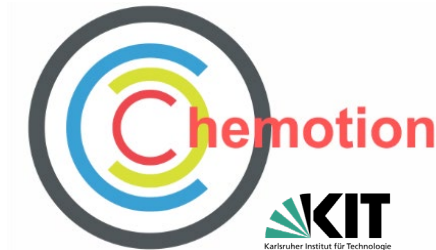
ELN-Driven InteroperabilitY for **Metadata**



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Electronic lab journals (ELNs)

- ELNs are a key to systematic research data management
- support of scientific work
- enabling documentation, database and tool integration
- KIT and Hereon: development of discipline specific ELNs



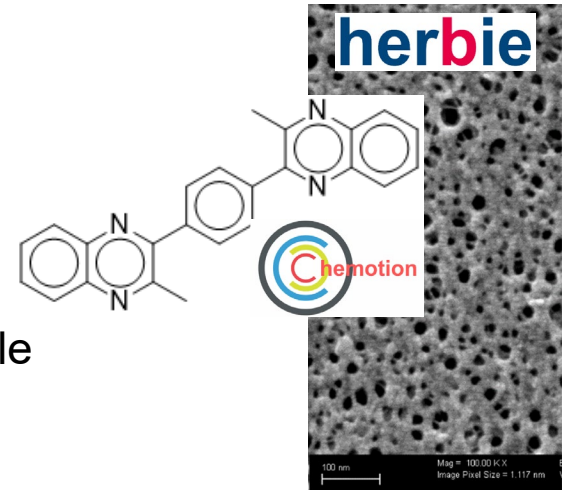
Problem: Missing interoperability

Aim:

- using multiple ELNs in one institution/project with (full) interoperability
- use case: Herbie and Chemotion
chemical post-modification of PAN-membranes

Current status:

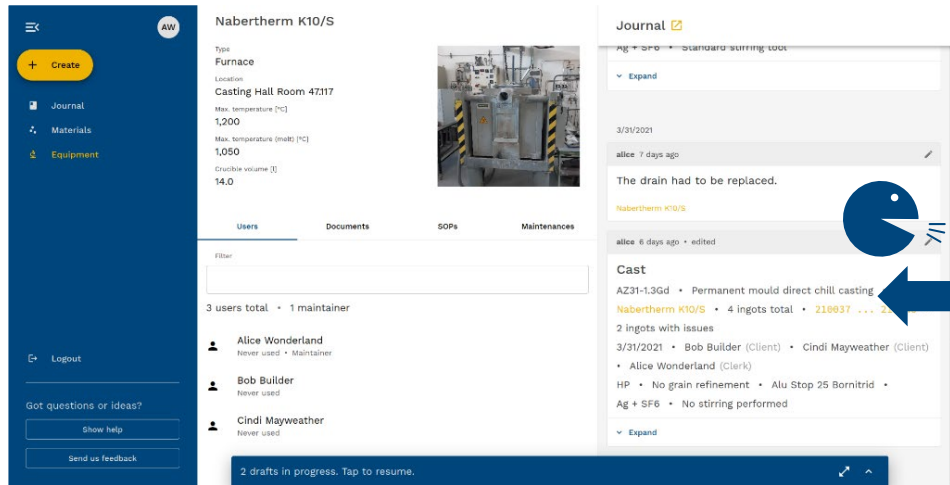
- collaborators use different ELNs
- interoperability between ELNs generally not available
-> hard to achieve for discipline specific ELNs



Solution: Metadata exchange package

Herbie

Chemotion



Nabertherm K10/S

Type: Furnace
Location: Casting Hall Room 47317
Max. temperature [°C]: 1,200
Max. temperature (melt) [°C]: 1,050
Crucible volume [l]: 14.0

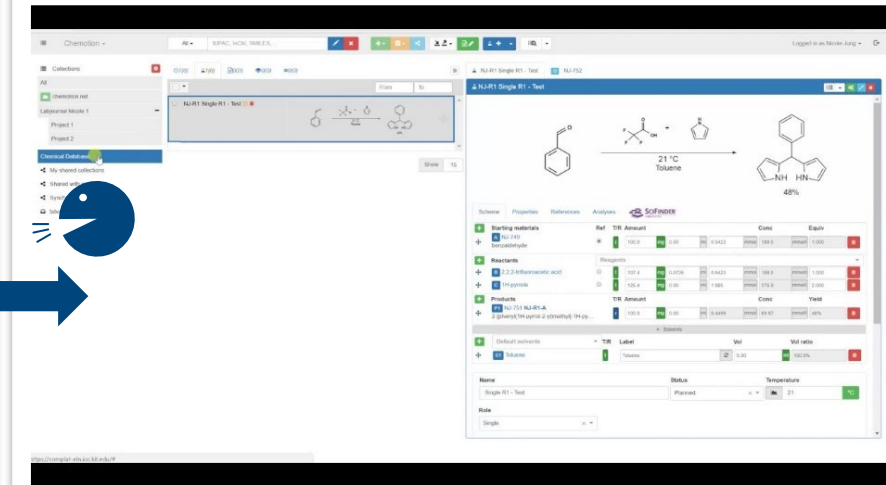
Users: Alice Wonderland, Bob Builder, Cindi Mayweather

Journal

3/31/2021
alice 7 days ago
The drain had to be replaced.

alice 6 days ago • edited

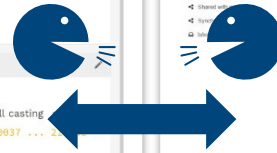
Cast
AZ31-1.3Gd • Permanent mould direct chill casting
Nabertherm K10/S • 4 ingots total • 210037 ... 2
2 ingots with issues
3/31/2021 • Bob Builder (Client) • Cindi Mayweather (Client) • Alice Wonderland (Clerk)
HP • No grain refinement • Alu Stop 25 Boronitrid • Ag + SF6 • No stirring performed



Chemotion

Reaction: c1ccc(cc1)C(=O)O + c1ccc(cc1)O >> c1ccc(cc1)Nc2ccc(cc2)N
21 °C
Toluene
48%

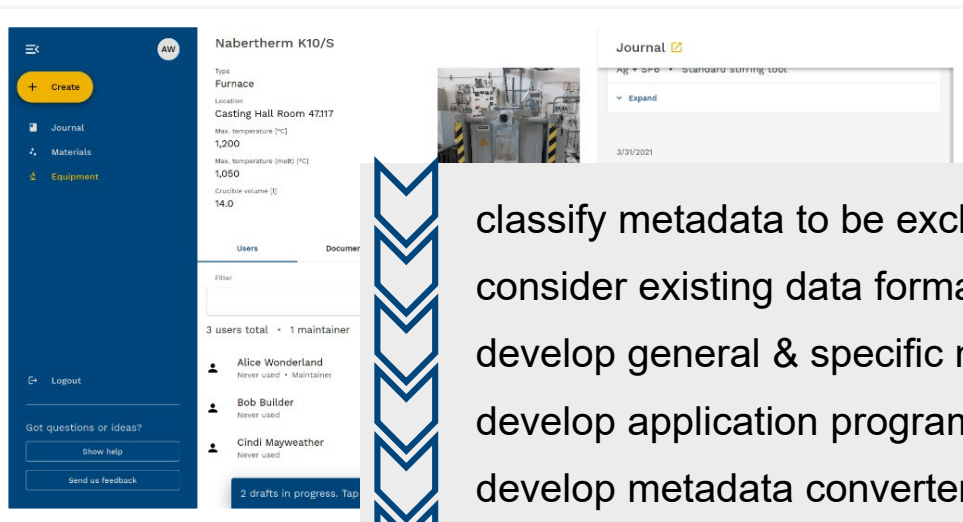
Starting materials	Ref	TIR Amount	Cost	Equip
100 g Toluene	100.0	1.000	1.000	1.000
2.0 g Acetic acid	2.0	0.020	0.020	0.020
100 g Toluene	100.0	1.000	1.000	1.000
100 g Toluene	100.0	1.000	1.000	1.000



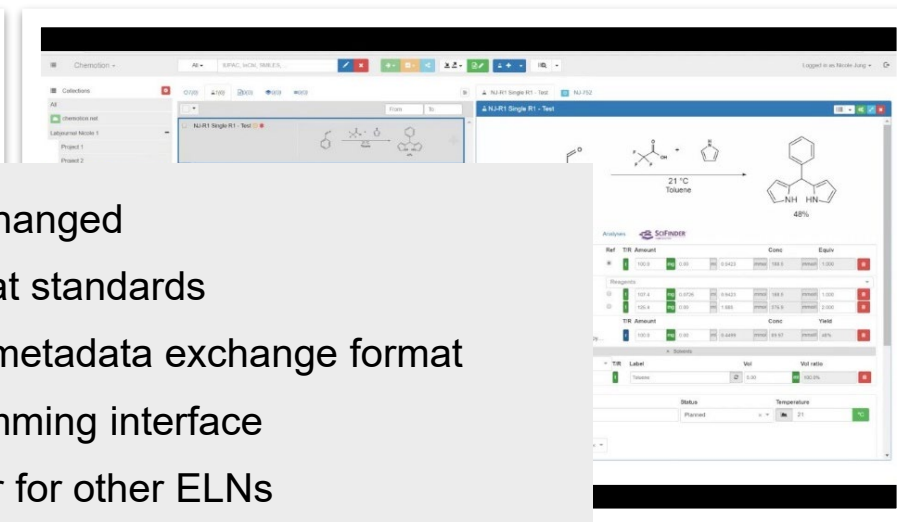
Solution: Metadata exchange package

Herbie

Chemotion



The screenshot shows the Herbie interface for a Nabertherm K10/S furnace. The left sidebar contains navigation options: Create, Journal, Materials, and Equipment. The main content area displays the furnace's location (Casting Hall Room 47317), maximum temperatures (1,200°C and 1,050°C), and crucible volume (14.0). A list of users is shown, including Alice Wonderland, Bob Builder, and Cindi Mayweather. A status bar at the bottom indicates '2 drafts in progress. Tap'.



The screenshot shows the Chemotion interface. It features a chemical reaction scheme for the synthesis of a pyridine derivative at 21°C in toluene, yielding 48%. Below the reaction, there is a table of analysis results from Software.

Ref	TIR	Amount	Comp	Equip
1	100.0	1.00	1.000	1.000
2	100.0	1.00	1.000	1.000
3	100.0	1.00	1.000	1.000
4	100.0	1.00	1.000	1.000

classify metadata to be exchanged
 consider existing data format standards
 develop general & specific metadata exchange format
 develop application programming interface
 develop metadata converter for other ELNs
 publish guide

Support by and linkage to HMC

- support for distribution of the metadata exchange package and guideline
- support for advertisement
- communication with the community and data science experts
 - feedback & input by other centers
 - foster collaborations and further implementation

Thank You!

ELN-Driven Interoperability for Metadata



Helmholtz-Zentrum
hereon