Boehringer Ingelheim

PSDI Autrans, 29-31.10.2007

ELIAS,

the Electronic Laboratory Information and Archiving System

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What ELIAS is:

- ELIAS is a workflow software which was developed to represent the processes within the Biberach structural research group.

- The emphasis is on the exchange of information between all automation systems and the electronic laboratory notebook system.

The aim of the project is to

- enable every member of the group to track all information on a certain sample.
- Simplify “high througput crystallography”

System overview

ELIAS
SR-databases
other databases

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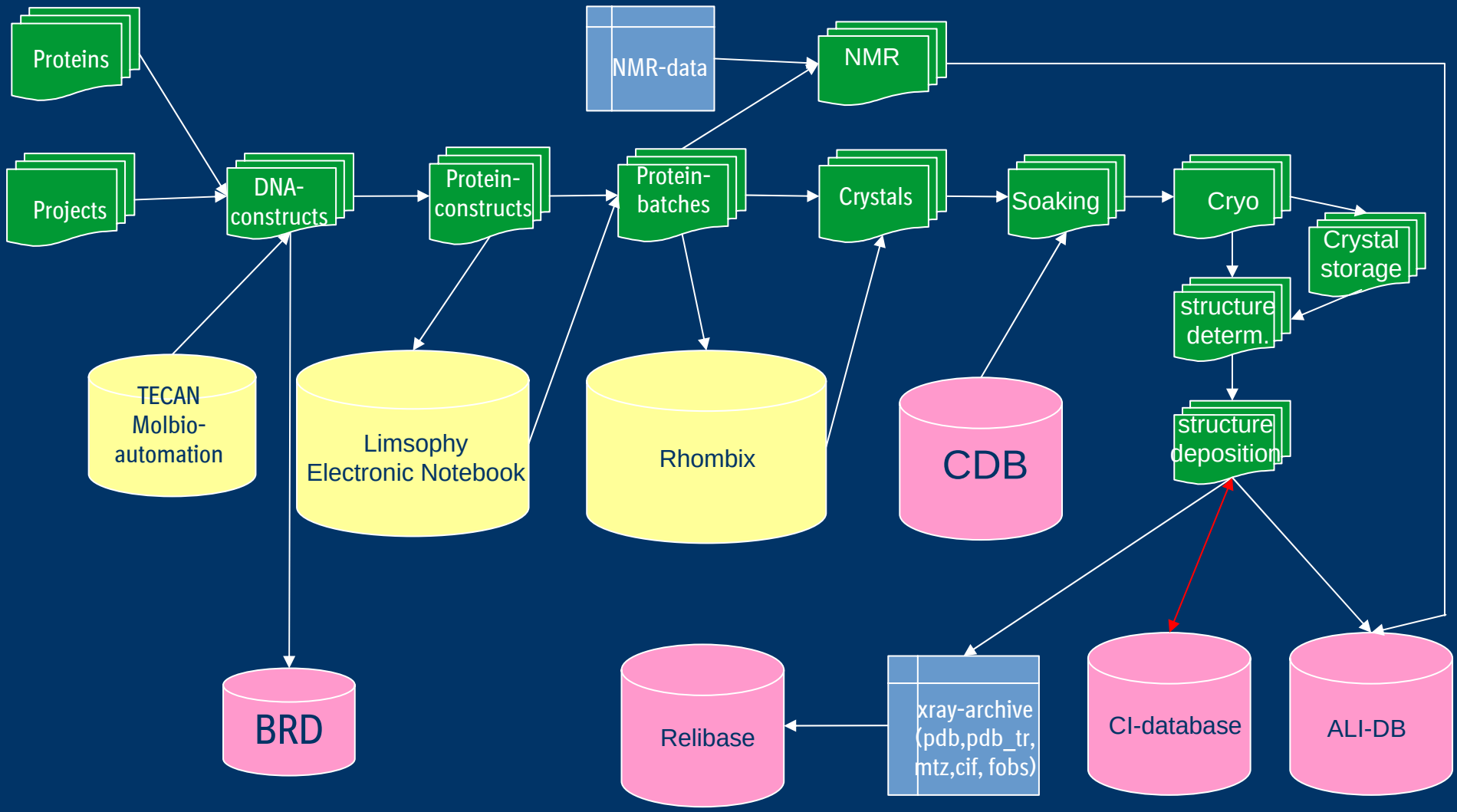
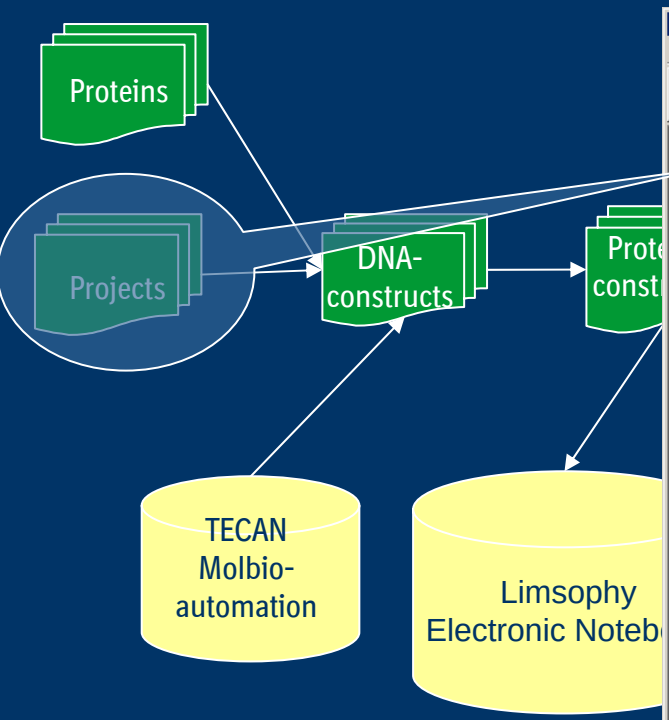
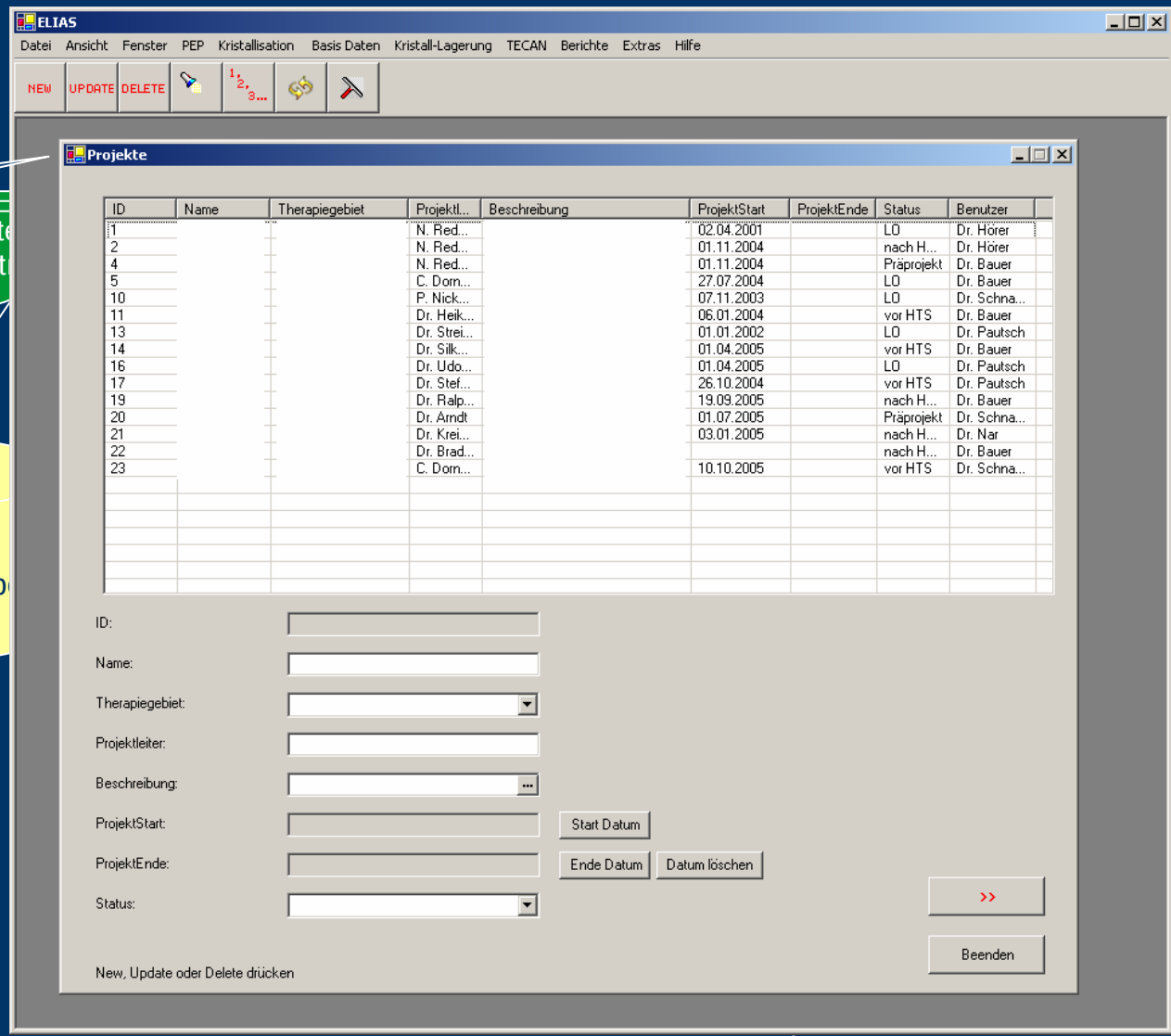


ELIAS workflow (1)
Projects





ELIAS workflow (2)
DNA and protein constructs

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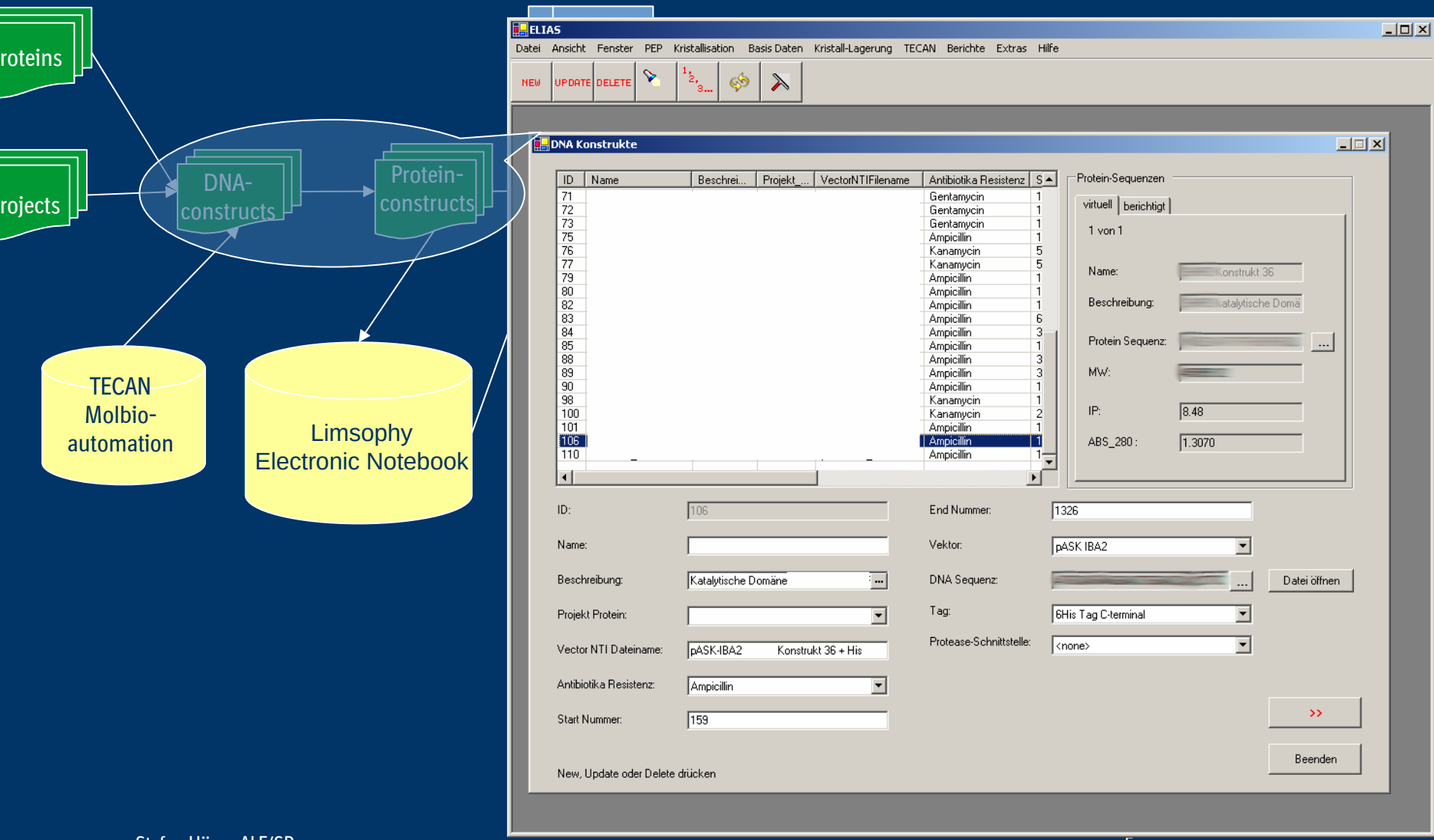

ELIAS workflow (3)
protein batches

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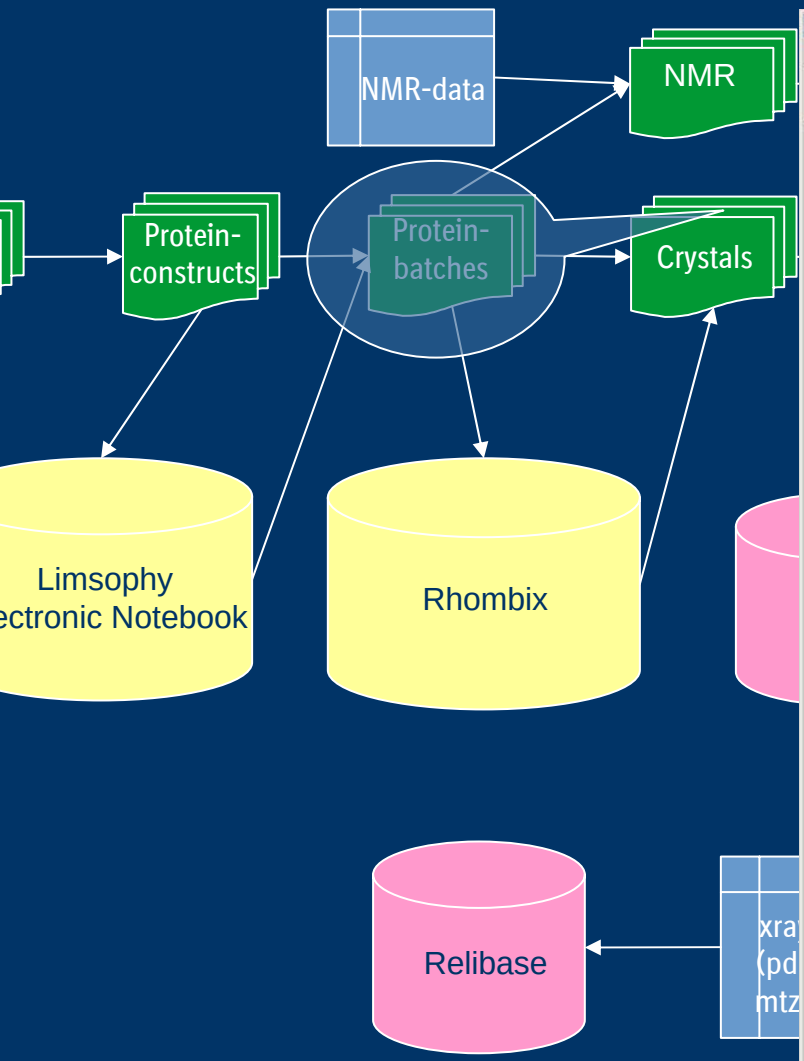

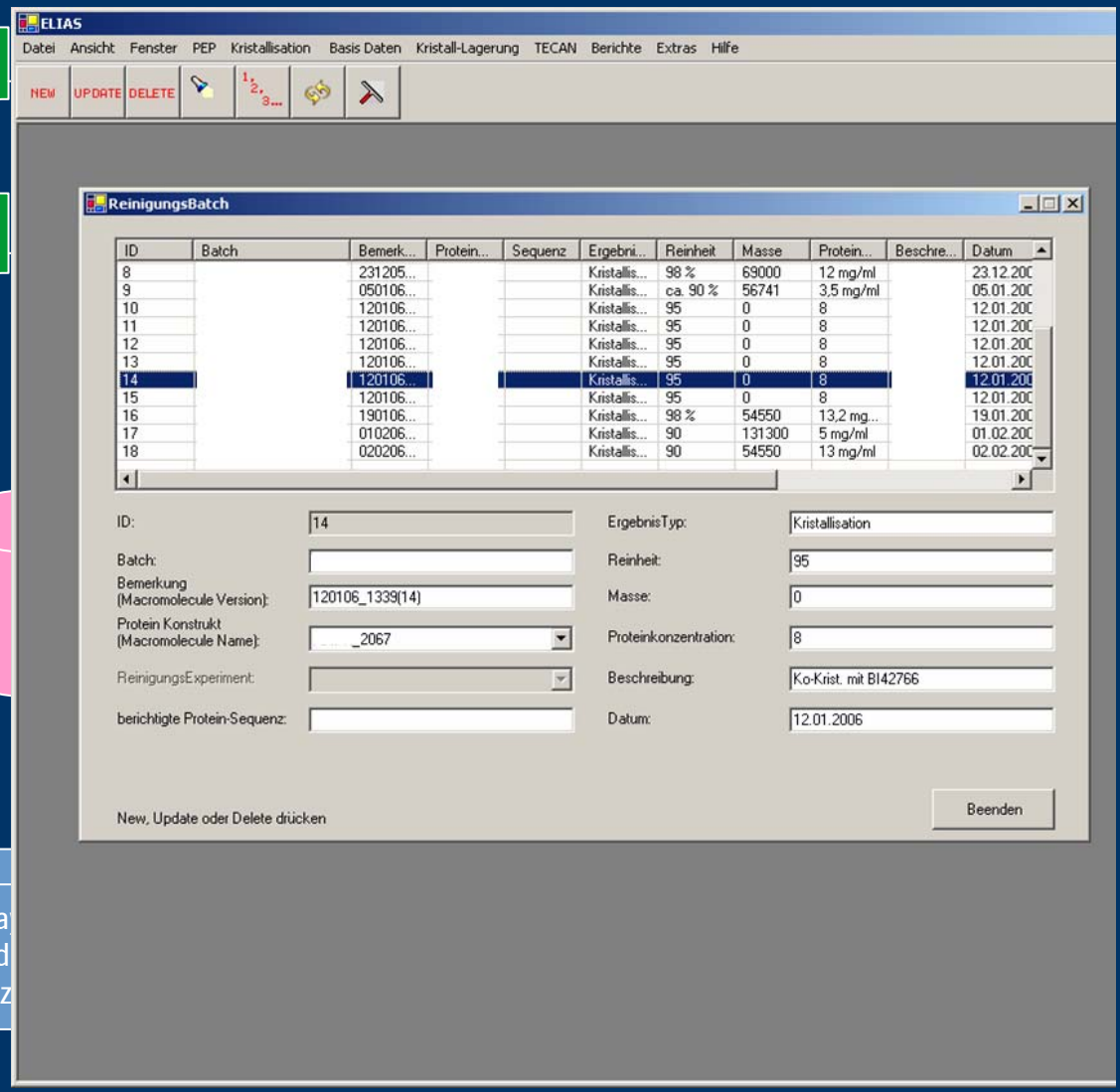

ELIAS workflow (4)
Crystals

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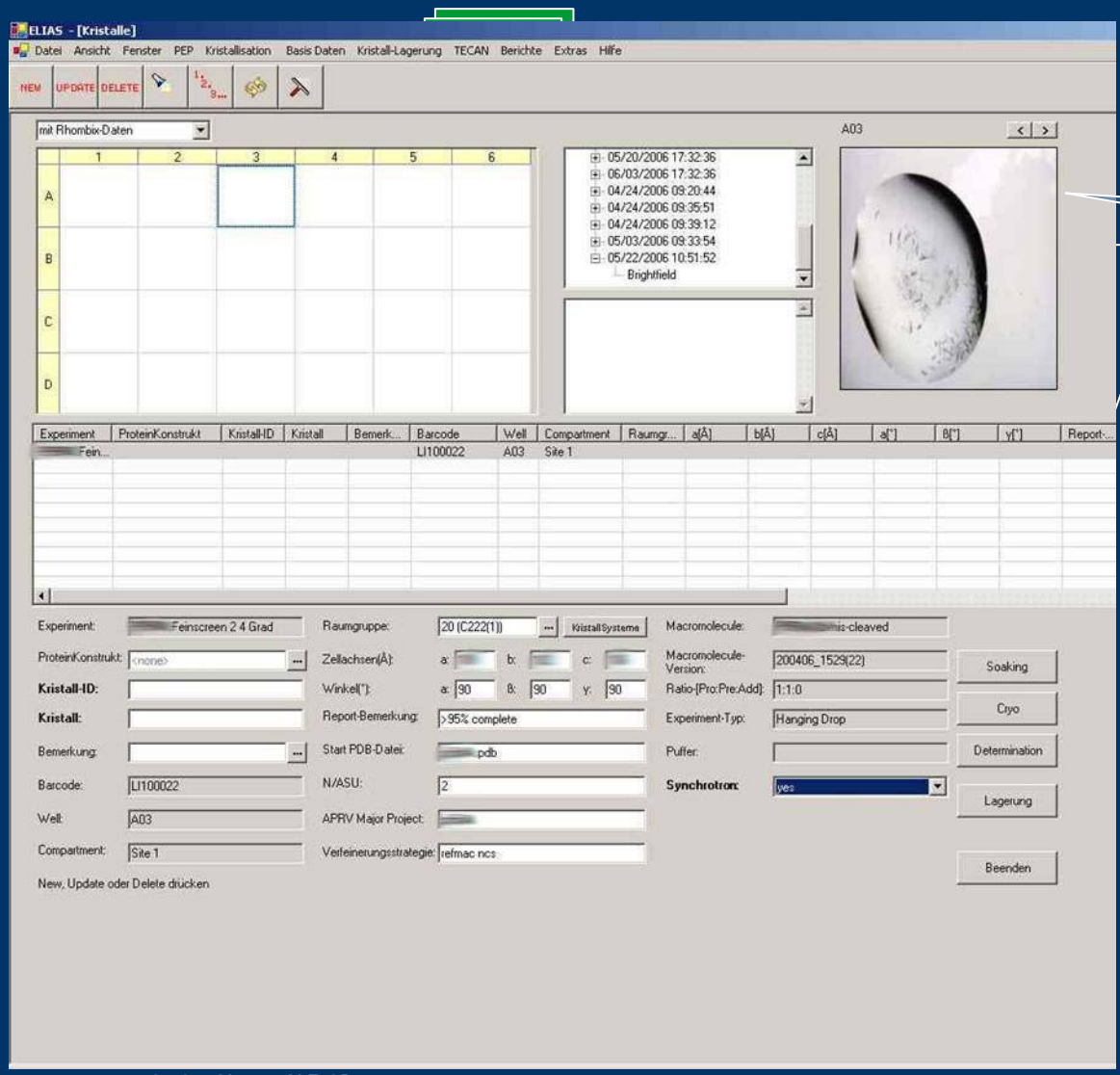

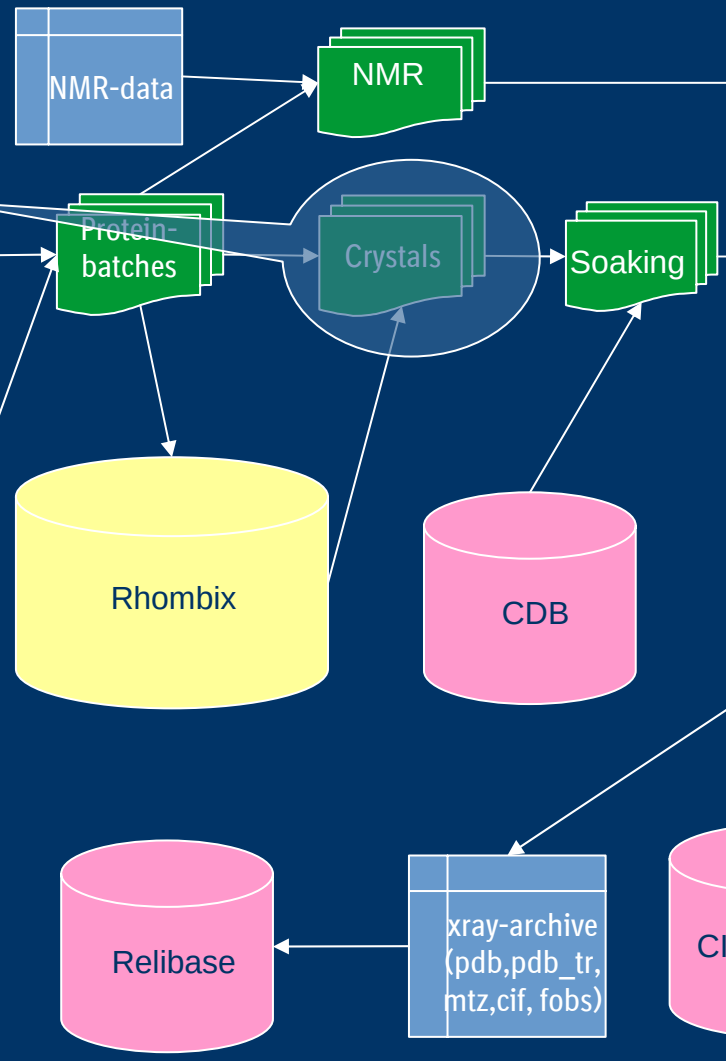

Soaking, Cryo, Storage

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Soaking:

- Biological assay data is loaded from the CDB
- a detailed soaking protocol can be stored as a method

Cryo:

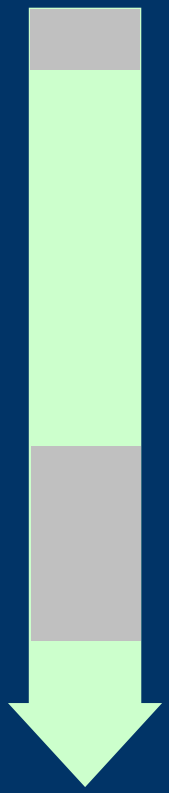
- Cryo-conditions can be tracked when optimizing a cryo-protocol

Storage:

- A storage position can be assigned to a crystal
  ⇨Reports for synchrotron trips

HTX Automation

current workflow



- data collection
- setup of data processing and refinement (information retrieved from ELIAS)
- data processing
- initial refinement
- setup of ligand and ligand libraries (information retrieved from ELIAS and CDB)
- ligand fitting, water picking and refinement
- manual inspection, rebuilding of protein and / or ligand
- further refinement
- validation
- deposition to ELIAS and RELIBASE

automatic process

manual process

HTX Automation

current workflow

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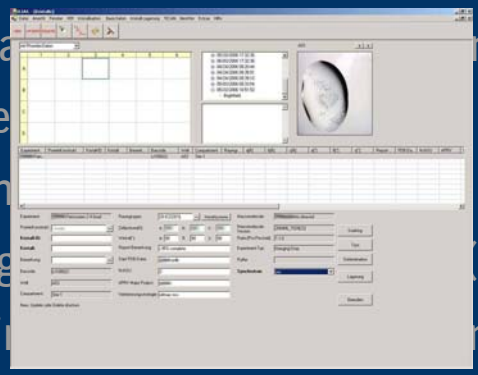
- data collection on Friday
- setu of da ment (informatio
- data proce
- initial refin
- setup of lig (information retrie
- ligand fitti nement
- manual inspection, rebuilding of protein and / or ligand on Monday
- further refinement
- validation



- deposition to ELIAS and RELIBASE

automatic process

manual process

Structure Deposition

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1. Selection of the files to deposit (pdb,mtz,cif,mol)
2. Generation of the pdb-file header
   Header is assembled from data stored for the specified crystal
3. Shell scripts generate the final pdb-file
4. Files are deposited to a network-drive
5. ELIAS stores the final files
6. Cronjob stores them to Relibase

Data exchange with other databases

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Relibase (CCDC):
Is the tool within BI to exchange structures between sites.

CDB (compound database):
ELIAS retrieves assay data available for compounds.

BRD (biological reagents database):
Stores all bioreagents available BI worldwide.
ELIAS reports DNA-constructs.

ALI-DB (alternative lead identification):
Global initiative to enable fragment based screening for all sites.
ELIAS reports NMR and X-ray experiments.

CI-DB (chemoinformatics):
Has read access and can retrieve information on crystal structures.

Acknowledgement

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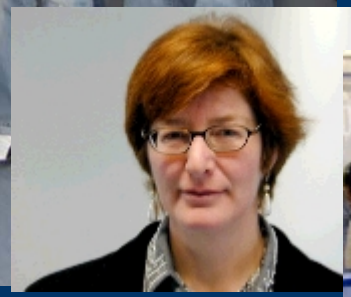

Stefan Hörer, ALF/SR