

PSDI Autrans, 29-31.10.2007

ELIAS,
the Electronic Laboratory Information and Archiving System

Tatjana Köhler (information systems department)

Stefan Hörer
Dirk Reinert

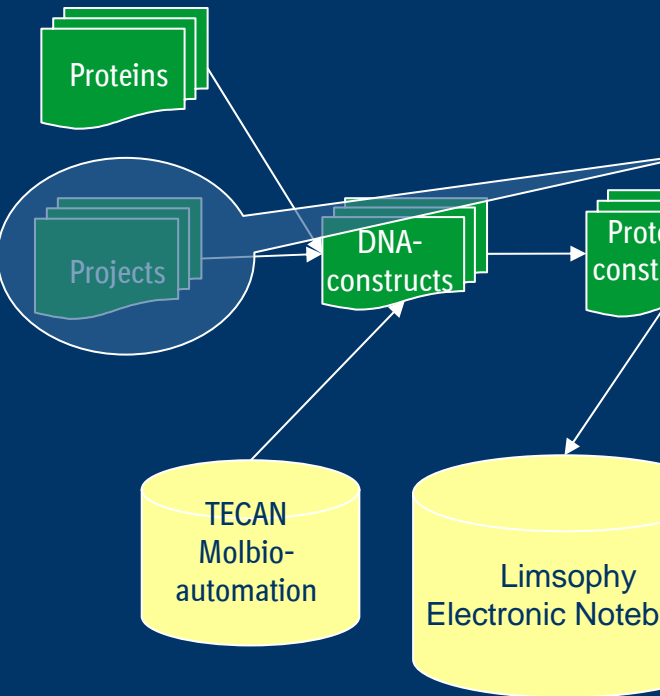
What ELIAS is:

- 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 throughput crystallography”

ELIAS workflow (1) Projects



ELIAS

Datei Ansicht Fenster PEP Kristallisation Basis Daten Kristall-Lagerung TECAN Berichte Extras Hilfe

NEW UPDATE DELETE

1 2 3...

Projekte

ID	Name	Therapiegebiet	Projekt...	Beschreibung	ProjektStart	ProjektEnde	Status	Benutzer
1			N. Red...		02.04.2001		LO	Dr. Hörer
2			N. Red...		01.11.2004		nach H...	Dr. Hörer
4			N. Red...		01.11.2004		Präprojekt	Dr. Bauer
5			C. Dorn...		27.07.2004		LO	Dr. Bauer
10			P. Nick...		07.11.2003		LO	Dr. Schna...
11			Dr. Heik...		06.01.2004		vor HTS	Dr. Bauer
13			Dr. Strei...		01.01.2002		LO	Dr. Pautsch
14			Dr. Silk...		01.04.2005		vor HTS	Dr. Bauer
16			Dr. Udo...		01.04.2005		LO	Dr. Pautsch
17			Dr. Stef...		26.10.2004		vor HTS	Dr. Pautsch
19			Dr. Ralp...		19.09.2005		nach H...	Dr. Bauer
20			Dr. Arndt		01.07.2005		Präprojekt	Dr. Schna...
21			Dr. Krei...		03.01.2005		nach H...	Dr. Nar
22			Dr. Brad...				nach H...	Dr. Bauer
23			C. Dorn...		10.10.2005		vor HTS	Dr. Schna...

ID:

Name:

Therapiegebiet:

Projektleiter:

Beschreibung:

ProjektStart: Start Datum

ProjektEnde: Ende Datum Datum löschen

Status:

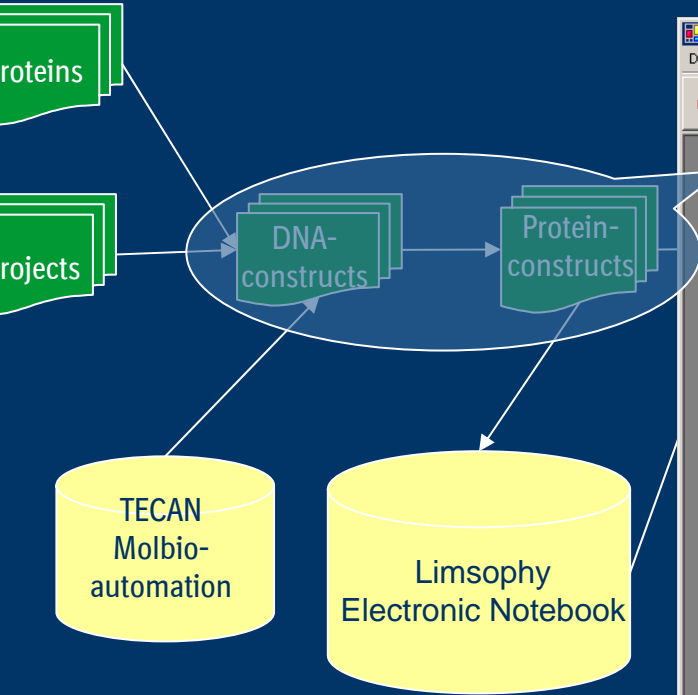
>>

Beenden

New, Update oder Delete drücken

ELIAS workflow (2)

DNA and protein constructs



ELIAS

Datei Ansicht Fenster PEP Kristallisation Basis Daten Kristall-Lagerung TECAN Berichte Extras Hilfe

NEW UPDATE DELETE

DNA Konstrukte

ID	Name	Beschrei...	Projekt...	VectorNTIFilename	Antibiotika Resistenz	S
71					Gentamycin	1
72					Gentamycin	1
73					Gentamycin	1
75					Ampicillin	1
76					Kanamycin	5
77					Kanamycin	5
79					Ampicillin	1
80					Ampicillin	1
82					Ampicillin	1
83					Ampicillin	6
84					Ampicillin	3
85					Ampicillin	1
88					Ampicillin	3
89					Ampicillin	3
90					Ampicillin	1
98					Kanamycin	1
100					Kanamycin	2
101					Ampicillin	1
106					Ampicillin	1
110					Ampicillin	1

Protein-Sequenzen

virtuell | berichtigt

1 von 1

Name:

Beschreibung:

Protein Sequenz:

MW:

IP:

ABS_280:

ID: End Nummer:

Name:

Beschreibung: ...

Projekt Protein:

Vector NTI Dateiname:

Antibiotika Resistenz:

Start Nummer:

End Nummer:

Vektor:

DNA Sequenz: Datei öffnen

Tag:

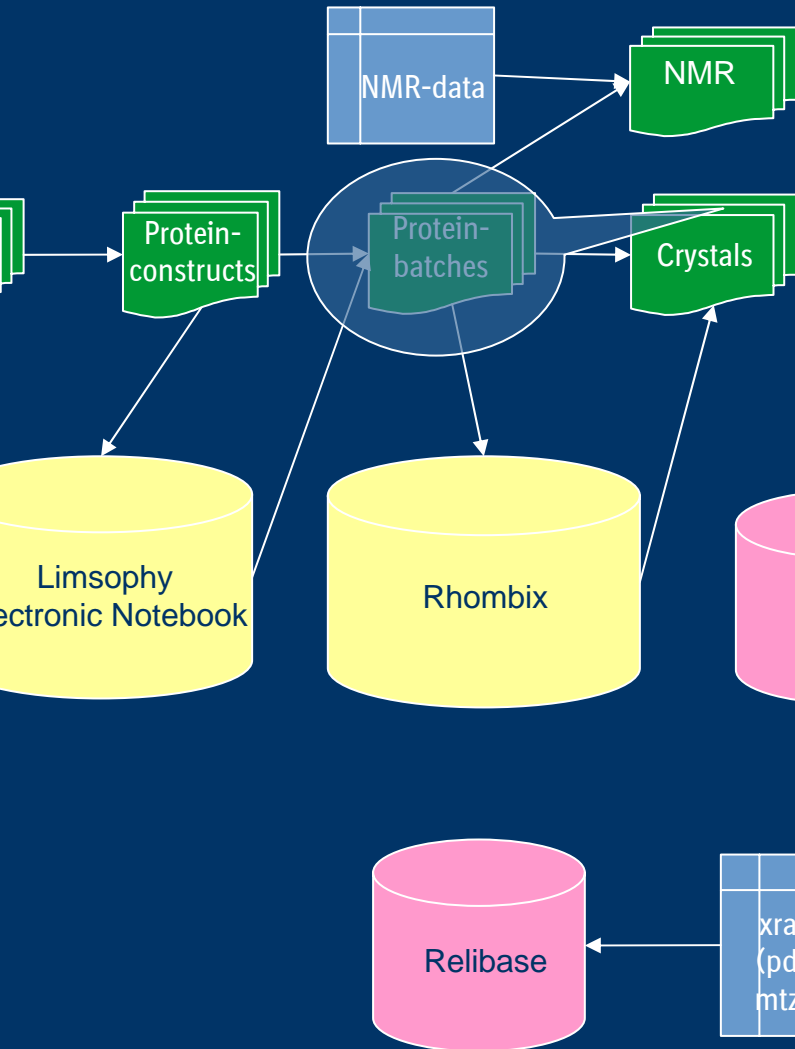
Protease-Schnittstelle:

>>

Beenden

New, Update oder Delete drücken

ELIAS workflow (3) protein batches



The screenshot shows the ELIAS software interface. The main window is titled "ReinigungsBatch" and contains a table of protein batches. The table has columns for ID, Batch, Bemerkung, Protein, Sequenz, Ergebnis, Reinheit, Masse, Protein, Beschreibung, and Datum. Row 14 is selected. Below the table is a form for editing the details of the selected batch (ID: 14).

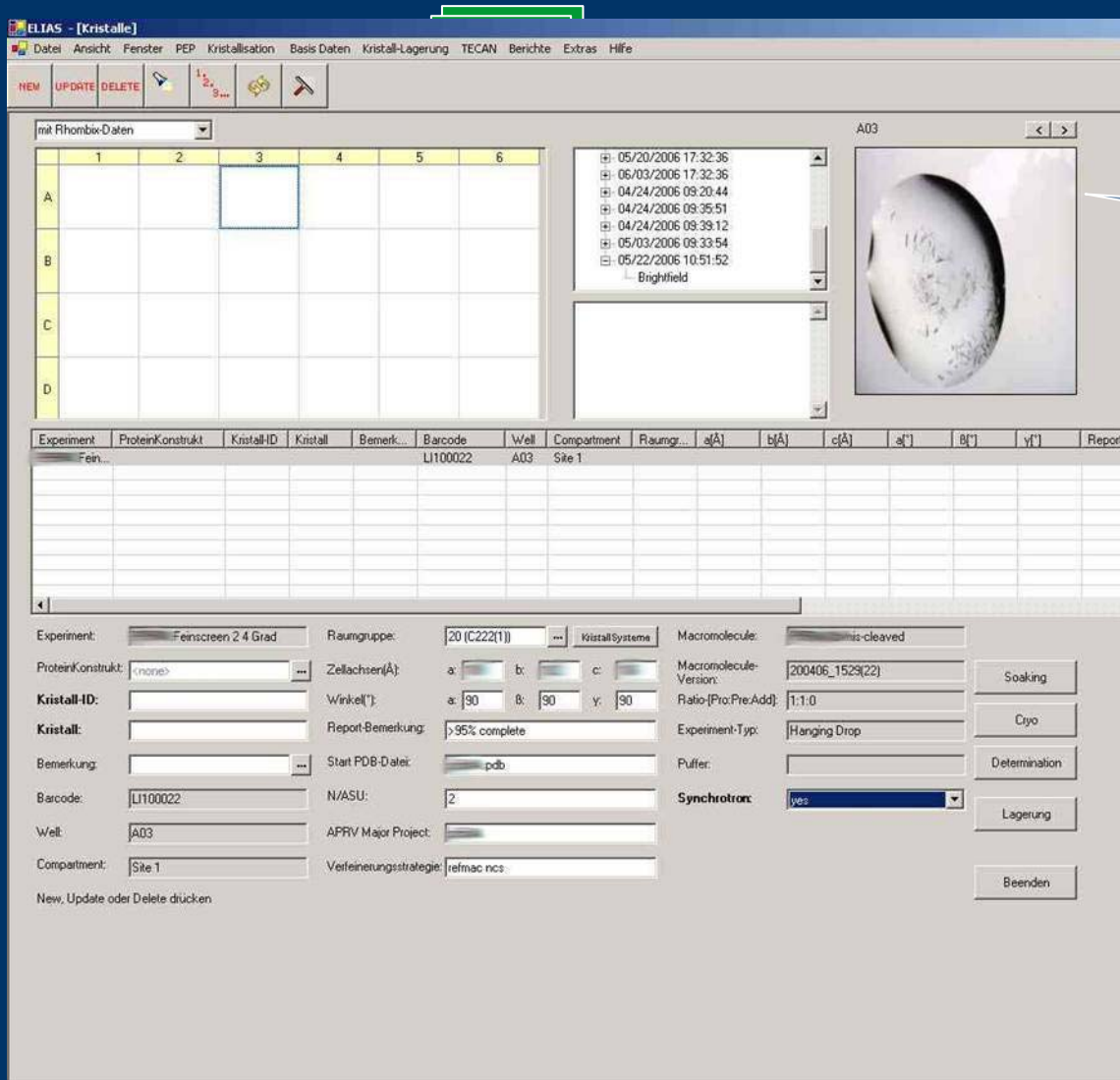
ID	Batch	Bemerkung	Protein	Sequenz	Ergebnis	Reinheit	Masse	Protein	Beschreibung	Datum
8		231205...			Kristallis...	98 %	69000	12 mg/ml		23.12.200
9		050106...			Kristallis...	ca. 90 %	56741	3,5 mg/ml		05.01.200
10		120106...			Kristallis...	95	0	8		12.01.200
11		120106...			Kristallis...	95	0	8		12.01.200
12		120106...			Kristallis...	95	0	8		12.01.200
13		120106...			Kristallis...	95	0	8		12.01.200
14		120106...			Kristallis...	95	0	8		12.01.200
15		120106...			Kristallis...	95	0	8		12.01.200
16		190106...			Kristallis...	98 %	54550	13,2 mg...		19.01.200
17		010206...			Kristallis...	90	131300	5 mg/ml		01.02.200
18		020206...			Kristallis...	90	54550	13 mg/ml		02.02.200

Form fields for ID: 14:

- ErgebnisTyp: Kristallisation
- Reinheit: 95
- Masse: 0
- Proteinkonzentration: 8
- Beschreibung: Ko-Krist. mit B142766
- Datum: 12.01.2006

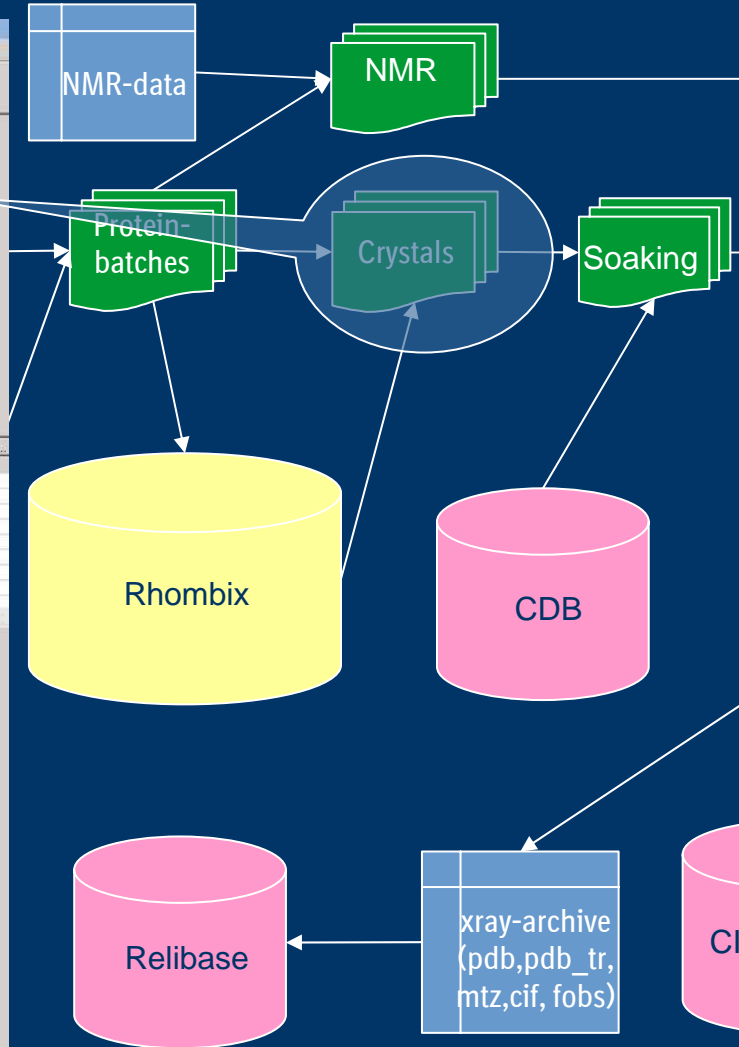
Buttons: NEW, UPDATE, DELETE, and a "Beenden" button.

ELIAS workflow (4) Crystals



The screenshot shows the ELIAS software interface with the following components:

- Table:** A table with columns 1-6 and rows A-D. Row 3, column 3 is highlighted.
- Image:** A circular image of a crystal labeled 'A03'.
- Configuration Fields:**
 - Experiment: Feinscreen 2.4 Grad
 - Proteinkonstrukt: <none>
 - Kristall-ID: <empty>
 - Kristall: <empty>
 - Bemerkung: <empty>
 - Barcode: LI100022
 - Well: A03
 - Compartment: Site 1
 - Raumgruppe: 20 (C222(1))
 - Zellachsen(Å): a, b, c
 - Winkel(°): a: 90, b: 90, c: 90
 - Report-Bemerkung: >95% complete
 - Start PDB-Datei: pdb
 - N/ASU: 2
 - Verfeinerungsstrategie: refmac ncs
 - Macromolecule: his-cleaved
 - Macromolecule-Version: 200406_1529(22)
 - Ratio(Pro:Pre:Add): 1:1:0
 - Experiment-Typ: Hanging Drop
 - Puffer: <empty>
 - Synchrotron: yes
- Buttons:** Soaking, Cryo, Determination, Lagerung, Beenden.



Soaking, Cryo, Storage

Soaking:

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

Cryo:

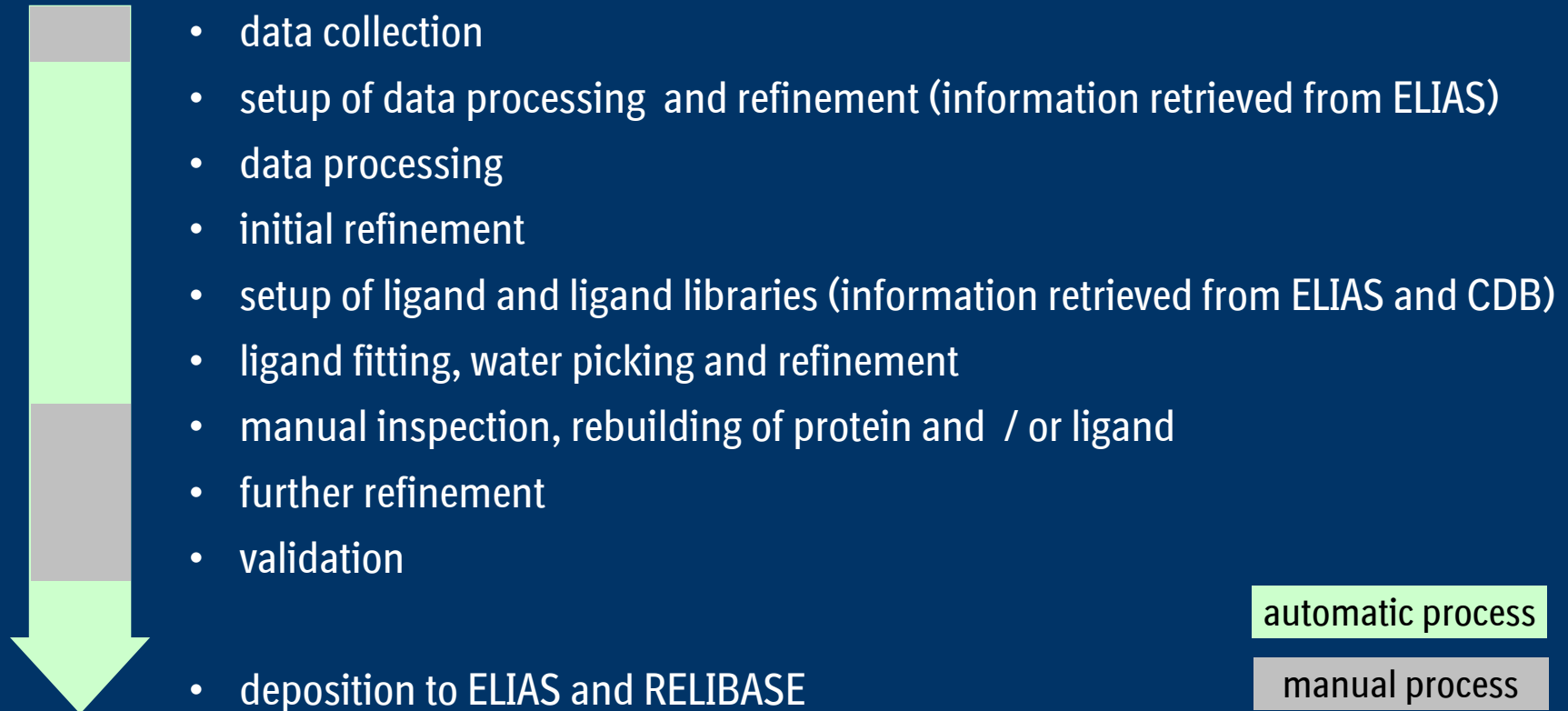
- Cryo-conditions can be tracked when optimizing a cryo-protocol

Storage:

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

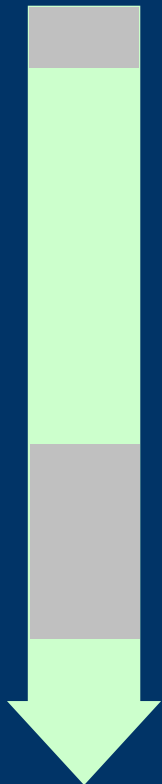
HTX Automation

current workflow

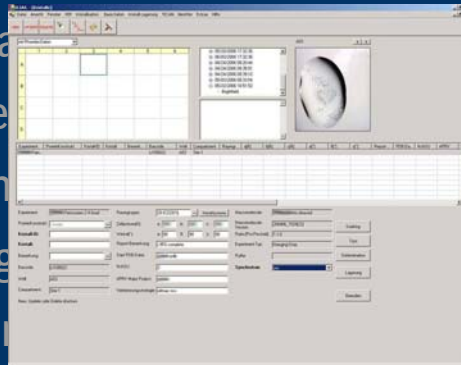


HTX Automation

current workflow



- data collection on Friday
- setup of data reduction (information retrieval)
- data processing (information retrieval)
- initial refinement (information retrieval)
- setup of ligand fitting (information retrieval)
- ligand fitting (information retrieval)
- manual inspection, rebuilding of protein and / or ligand on Monday
- further refinement
- validation
- deposition to ELIAS and RELIBASE



automatic process

manual process

Structure Deposition

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

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

