NanoCommons Knowledge Base

Biomax Informatics AG, www.biomax.com

- Munich headquartered
- Global customer base
- 20 years of experience
- 50 staff

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Director Project Management

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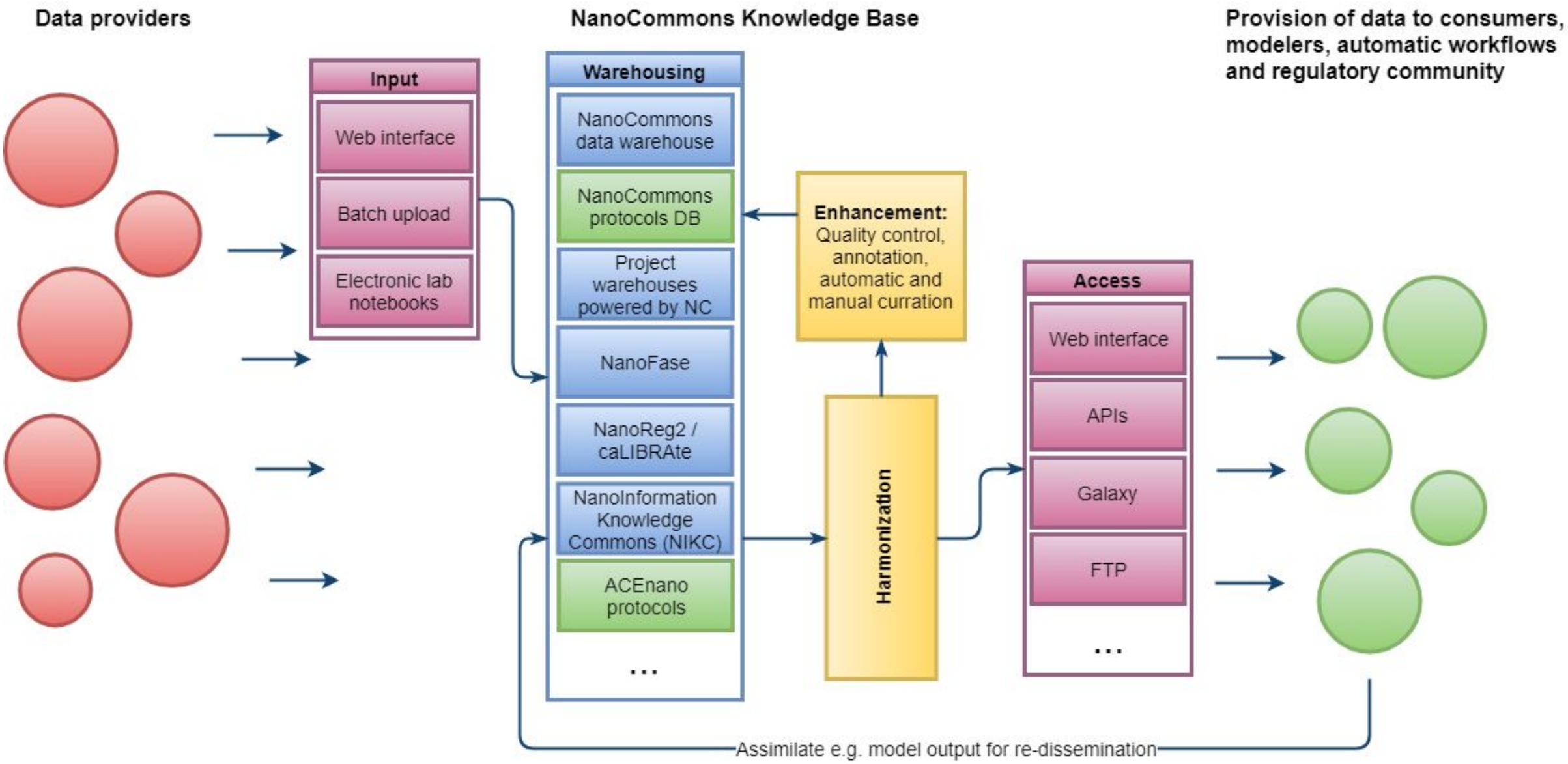
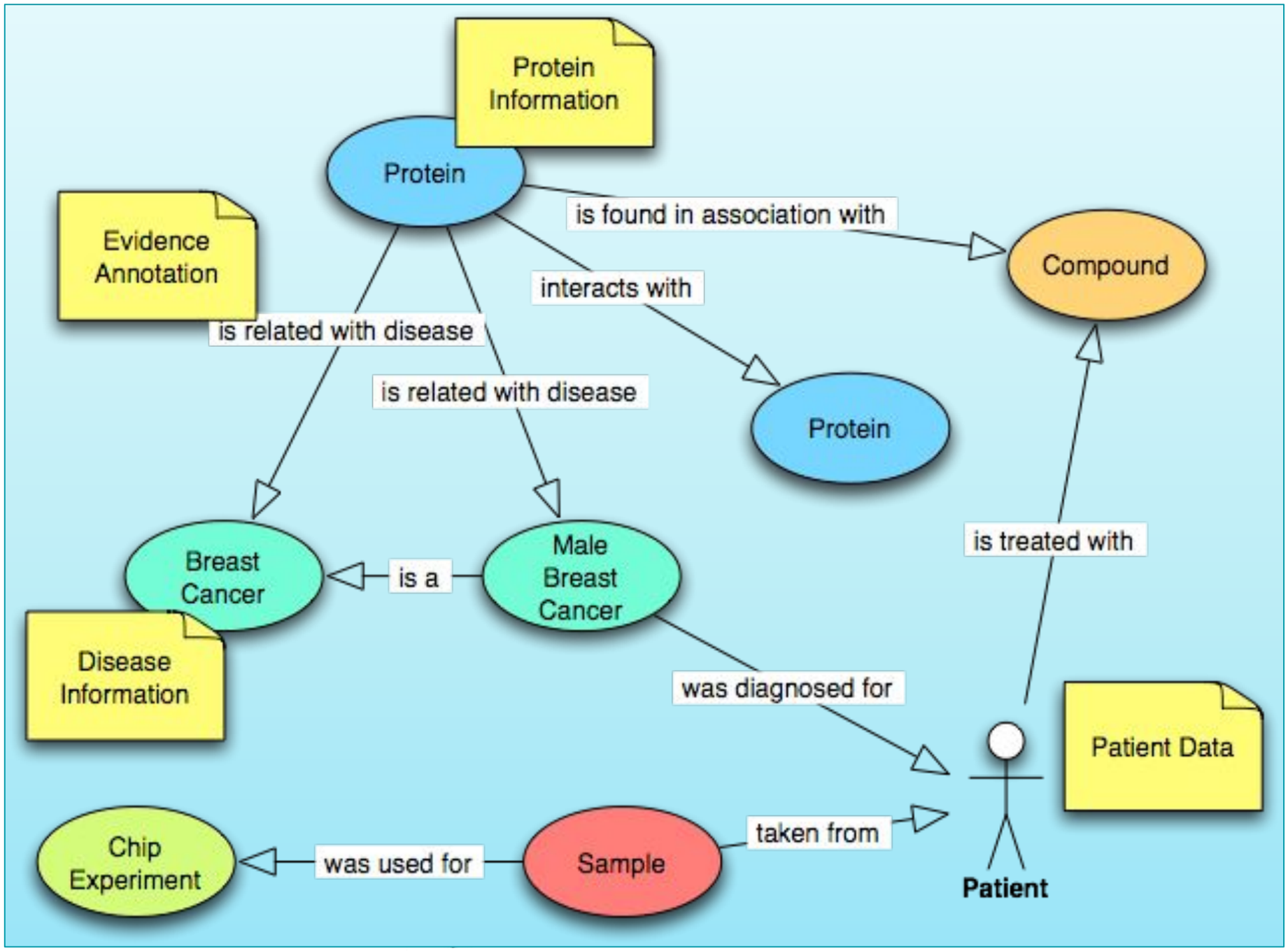
NanoCommons KB Architecture concept



Knowledge management - handling complexity

Semantic Model



Semantic Model for integration and interoperability

NanoCommons
Nano-Knowledge Community

Researcher — **Machine learning**

Modeller — **Model validation**

Regulator — **Approval**

Management — **Dash-boards**

UI ⇧ **API**

Query, analyse based on Semantic Model

Semantic Model

APIs

Semantically integrate any kind of data

Original data sources

NanoFASE
ENM eNanoMapper
ACEnano
NIKC
NanoMILE

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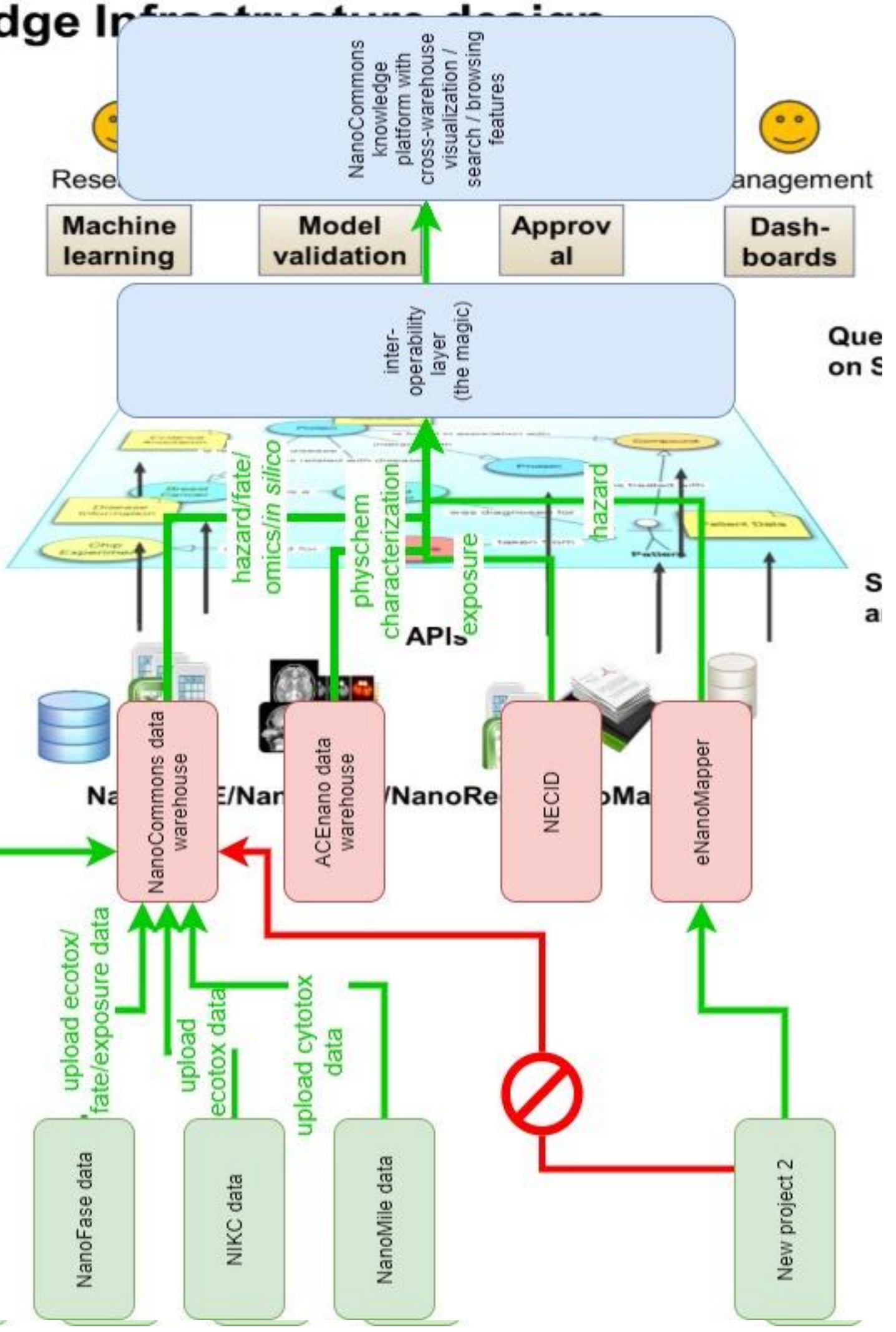
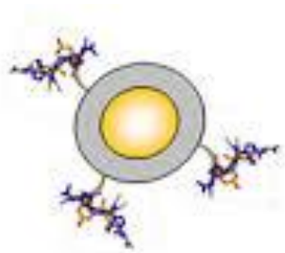
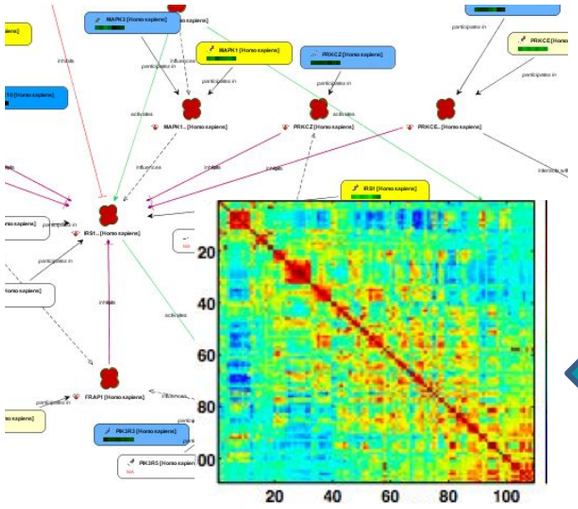
Knowledge In



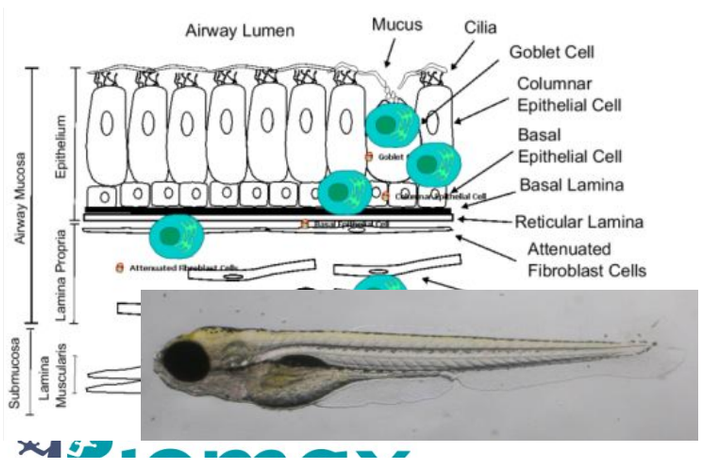
Coupling data and applications



Particle characterisation



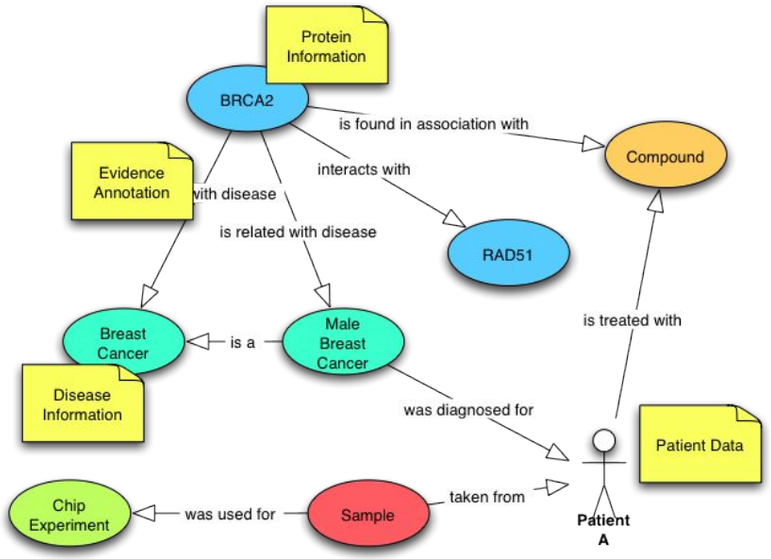
Molecular “omics” data and prior knowledge



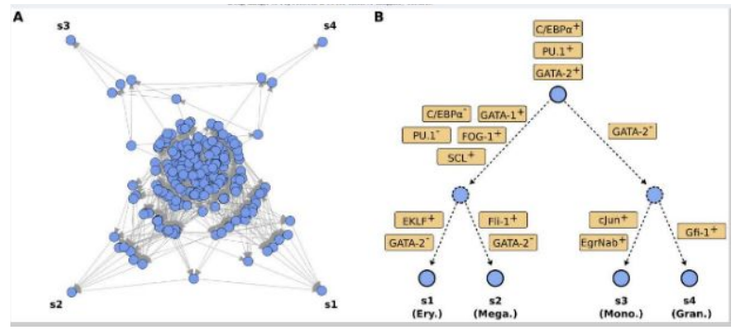
Classical Toxicology

Knowledge management

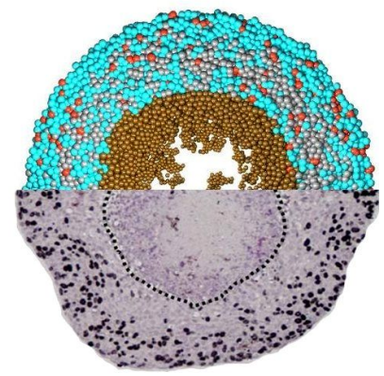
Semantic Model



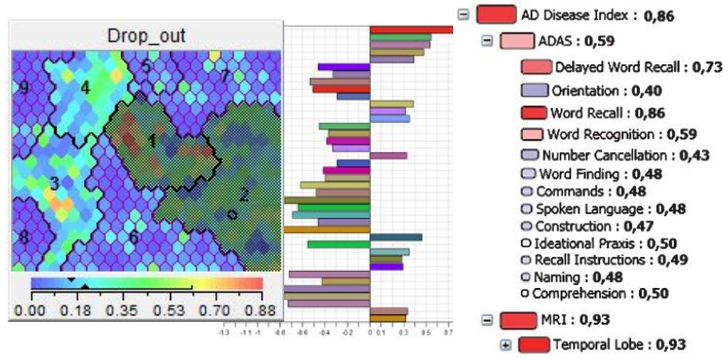
Network inference and data analysis



Computational Simulation



Biomarker profile



NanoCommons Knowledge Base - Content

NanoCommons
Nano-Knowledge Community

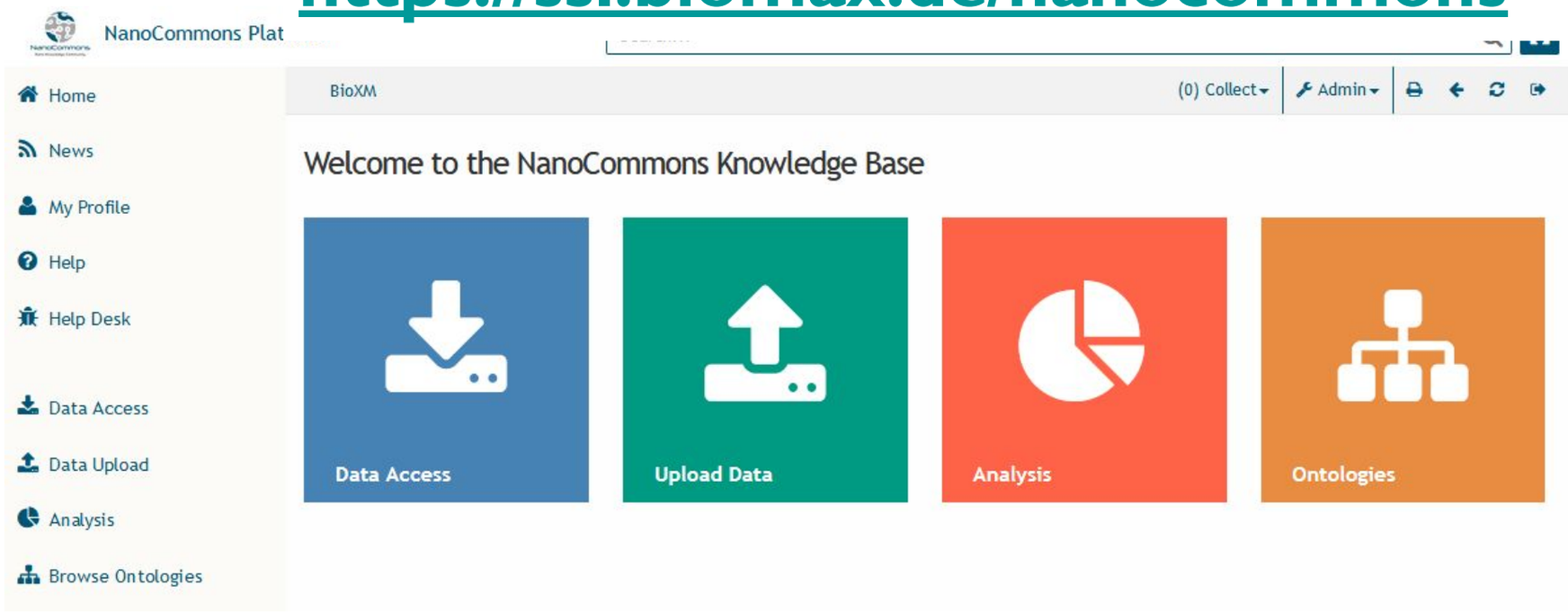
NanoMILE

NanoFASE
Fate and Exposure models for you - www.nanofase.eu

NanoCommons

NanoSolveIT

https://ssl.biomax.de/nanocommons



~500 Particles, Phys-Chem Characterisations, Protocols, Toxicology Experiments, Omics, Mesocosm from NanoMILE/NanoFASE

In-silico descriptors, Corona predictions, groupings, alerts from NanoCommons/NanoSolveIT

NanoMILE data is freely available, NanoFASE data is embargoed for 2 years (DTA available)
In-silico results come stepwise

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Tools

Knowledge Base with FAIR data

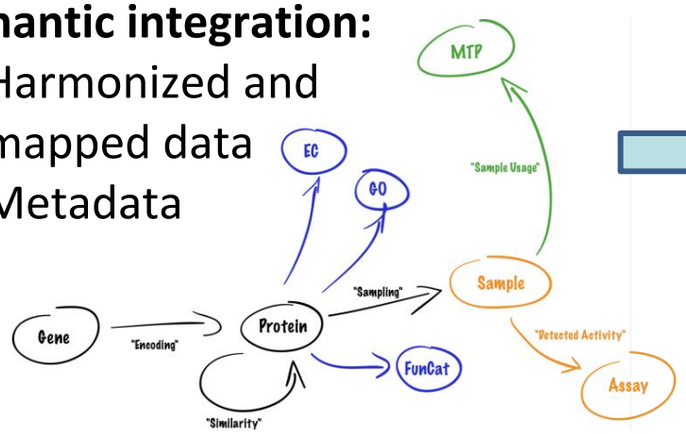
- Metadata fully searchable (including Ontologies e.g. NCBI Taxon, GO, eNMP)
- API based data access (Jaqpot)
- Generation of ontological descriptors for data
- Data upload
- Tool integration (Expression analysis, Modelling)

Data sustainability – beyond archives

Archive:
- Data store
- Metadata (Description)

Functions:
- Browse
- Search
- Retrieve
- Analyse

Semantic integration:
- Harmonized and mapped data
- Metadata



Functions:
- Navigate along connections
- Combine molecular, phenotype and environmental Information
- Visualize

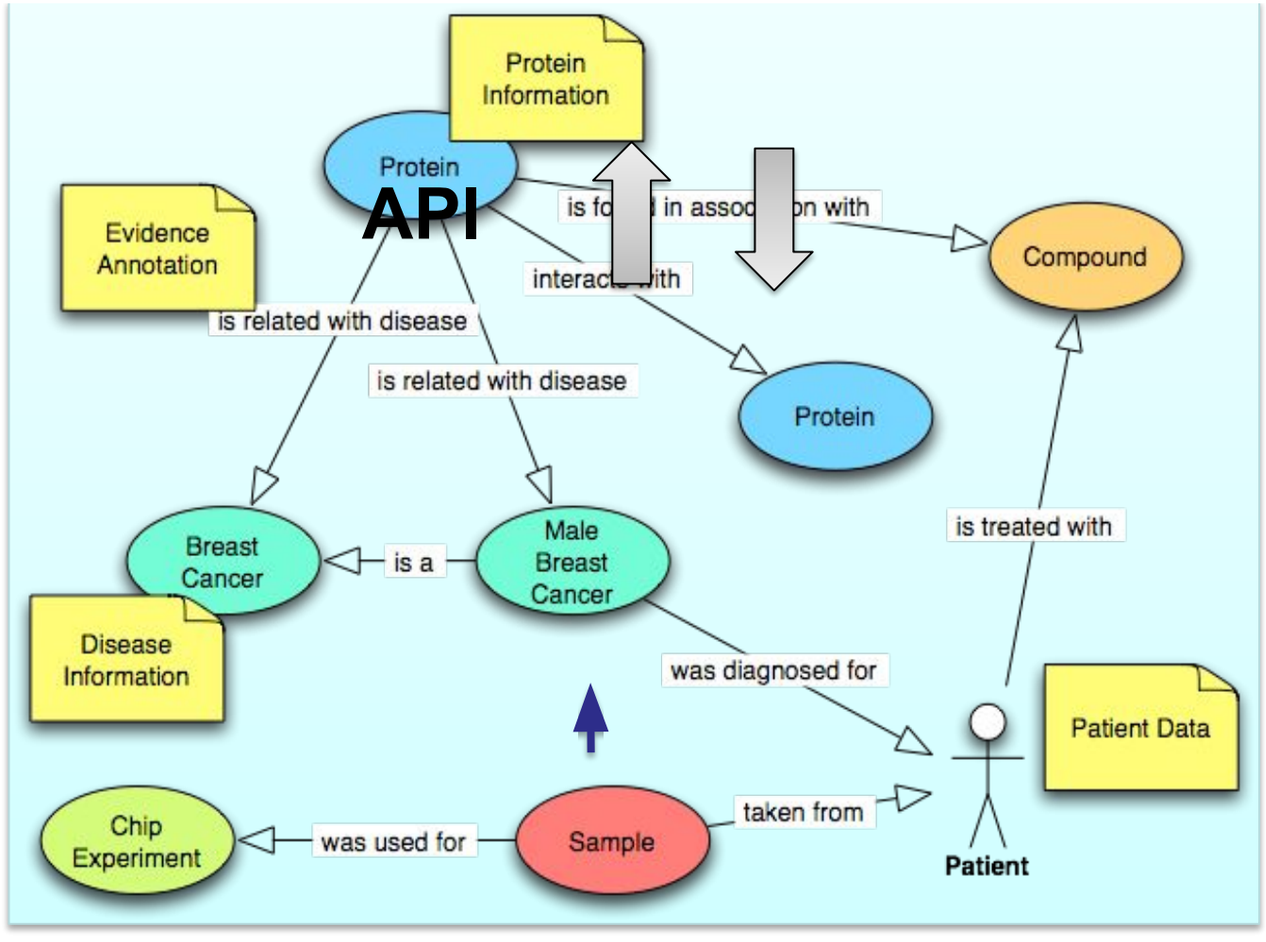
Example NanoMILE/NanoFASE knowledge base content:
- Genomes
- Pathways
- Protein-protein-interactions
- Transcription factor network
- Particles
- Orders/procurement
- Material safety sheets
- Ecotoxicological data
- ‘Omics

Integrated Services – Jaqpot REST Webservice

Knowledge Model for semantic interoperability e.g. Ontologies

API technical Interoperability

Integrated data sources



Query, analyse based on Knowledge Model

Semantically integrate any kind of data

Service – Data mining

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Nano-Knowledge Community

Particles

Particles Links

- View all Particles
- View Particles with Data

Toxicology

Toxicity Links

- View Toxicity Data sets
- View Toxicity Measurements by Data sets
- Search for Toxicity Measurements by Data set and Variables

BioXM » Characterisations

Actions | Export | (0) Collect | Admin

Excel
Tab delimited
Background exports

Particle Characterisation

Characterisation data

Nanoparticle | Search | + Add

Selected items: 2 | Show/Hide | Sort by

		Nominal size in dispersion [nm]	Nominal size as text	Minimal nominal size	Maximal nominal size	Shape	Crystallinity
	Nanoparticle	.	.	.	.	.	.
☑	NP00193	20.0 nm				Spherical	

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Service - Data upload and annotation

Download templates

Download Investigation Template

Upload templates

Upload Investigation Template

Datei | Start | Einfügen | Seitenlayout | Formeln

A4

	A	B
1	Add new Variable	eNanoMapper.Add new eNM ID
2	DLS (nm)	NPO_1469
3	PDI	NPO_1155
4		
5		

NanoCommons

Search...

dls

1 matches found

ENM:8000297 size_DLS

BFO:0000001 entity

BFO:0000019 quality

NPO_821 polydispersity

NPO_1697 size distribution

ENM:8000297 size_DLS

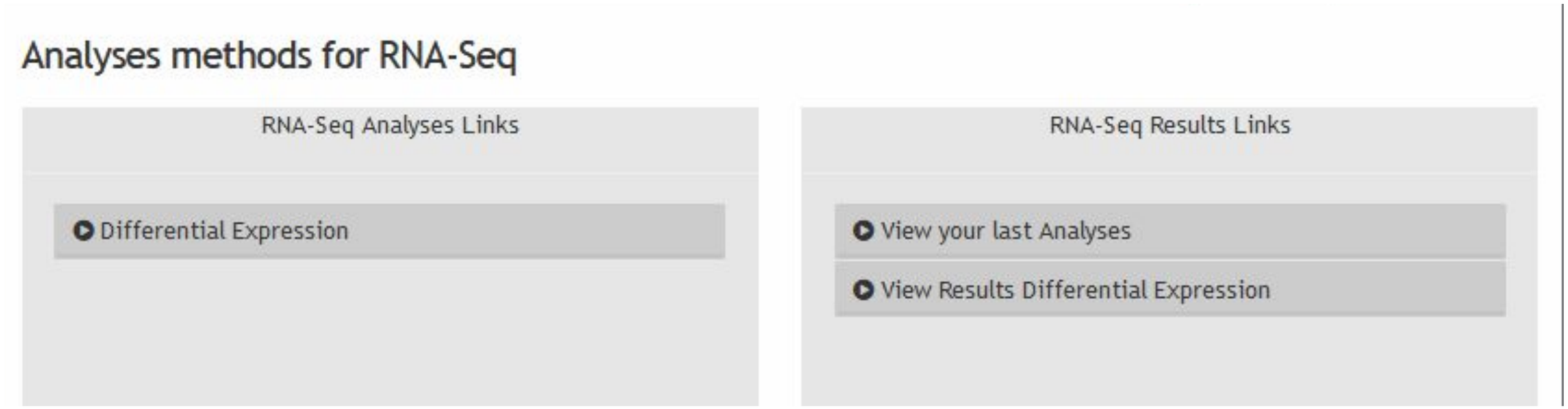
Download Investigation Template

Add new Variable | Search | + Add

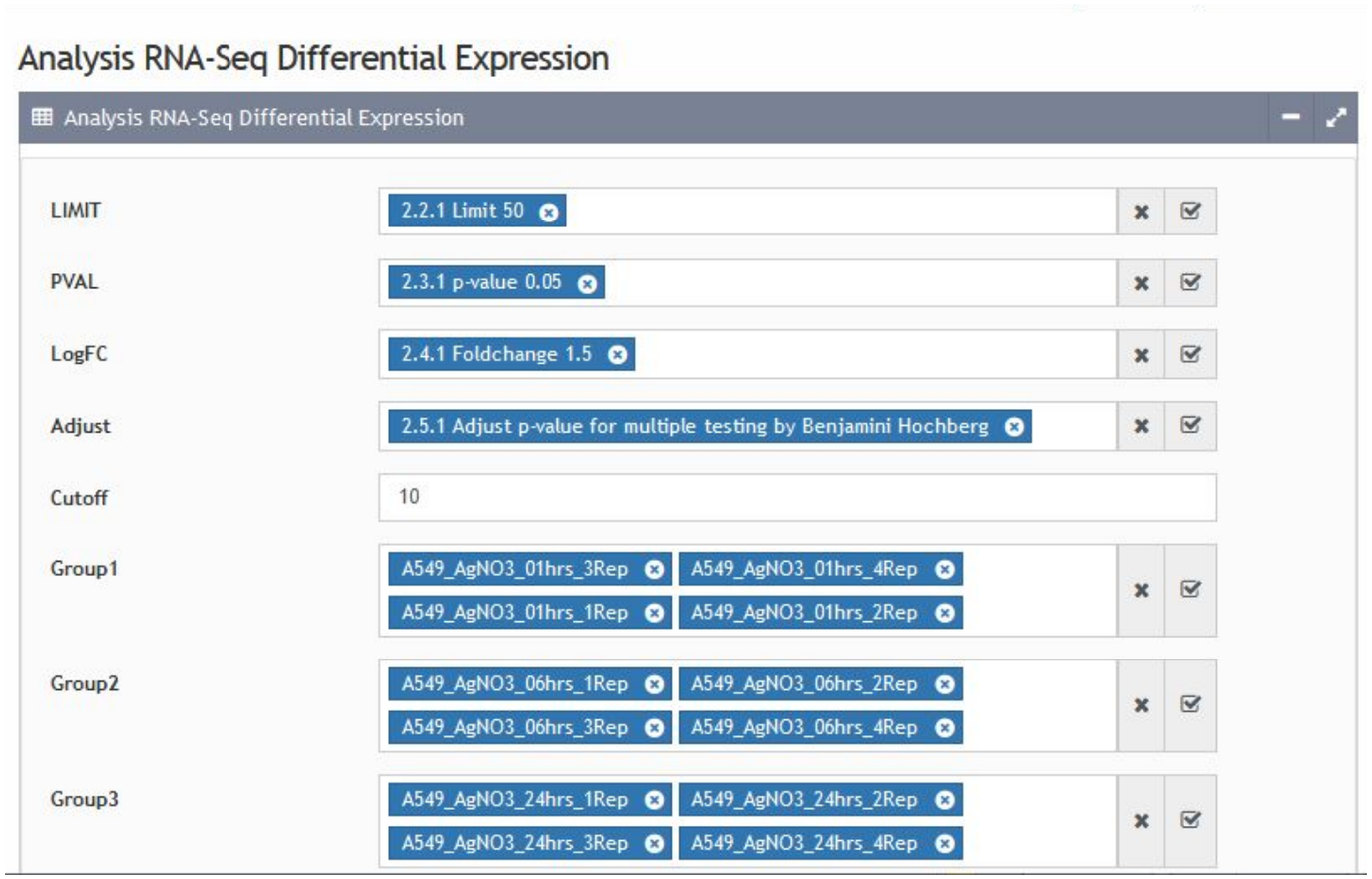
Selected items: 0 | Show/Hide | Sort by

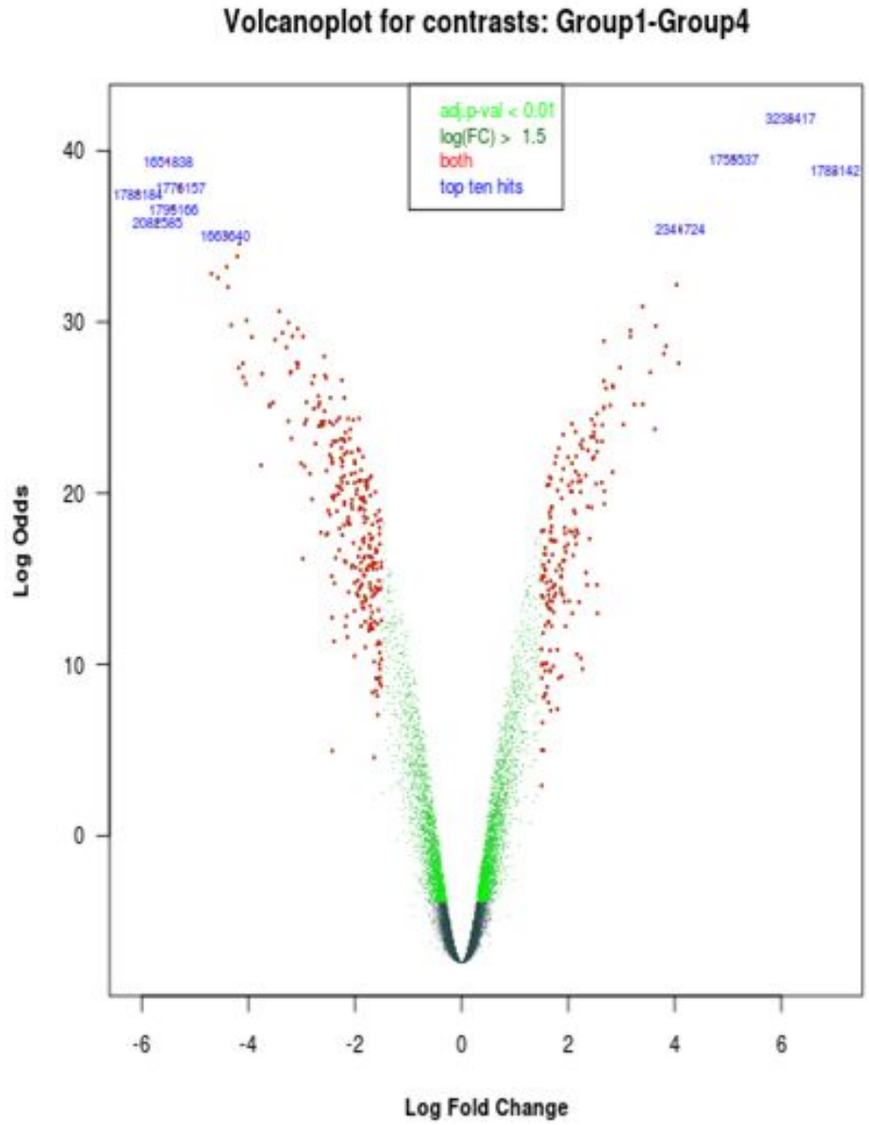
		eNanoMapper				
	Add new Variable	Add new eNM ID	Link	Name	Comment	Parents
⊕ ☐	DLS (nm)	NPO_1469	NPO_1469 dynamic light scattering	dynamic light scattering	[definition source: NCI]	FIX:0000402 light scattering; NPO_1712 light scattering spectroscopy

Integrated Services – Expression analysis



Integrated Services – Differential Expression analysis





Integrated Services – Corona model I

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Nano-Knowledge Community

Corona Analysis Overview

+ New Analysis Run | Task Manager

Per page: 25 Results: 4

Filter results by:

Analysis ID | Apply | + Add Filter

Show/Hide | Sort by

					Analysis Results	
Analysis ID	NanoParticle ID	Protein ID	Analysis Start	Started by User	Heatmap	Mapping
Analysis-0000000098	NP00477	Q9GU57	19.02.2020 13:49:22	martinz		1IXT_gold_12_16.map
Analysis-0000000102	NP00728	P04264	21.02.2020 18:17:13	dm_admin		6E2J_tio2_anatase_25_12.map
Analysis-0000000107	NP00478	Q16696	24.02.2020 09:46:18	martinz		3T3S_sio2_amorphious_12_-8.map
Analysis-0000000202	NP00477	Q9AHD4	28.02.2020 10:20:48	martinz		3QY8_gold_12_16.map

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Integrated Services – Corona model

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Select Input for **Analysis-0000000046**

Nanoparticle

Add | Remove

Protein

Add | Remove

Cancel Analysis

Add Objects

Results: 15 | Per page: 25

Names | au | Search | Add

Selected items: 0 | Show/Hide | Sort by

Particle ID	NanoFASE name	Designator	Names
NP00812	Au carboxylic acid-functionalized (JRC)		Au carboxylic acid-functionalized (JRC)
NP00811	Au amino-functionalized (JRC)		Au amino-functionalized (JRC)
NP00810	Au amino-functionalized (JRC)		Au amino-functionalized (JRC)
NP00809	Au pristine		Au pristine
NP00741			Au50-UoB;Au50-UoB Citrate capped
NP00740			Au20-UoB;Au20-UoB Citrate capped
NP00739			BBIAu80;BBIAu80-Citrate
NP00738			BBIAu60;BBIAu60-Citrate
NP00737			BBIAu20;BBIAu20-Citrate
NP00709	Aust-Ag2S	Aust-Ag2S	Aust-Ag2S
NP00480			Au_PEG-COOH;IO166E Gold 12 nm PEG-COOH
NP00479			Au_PEG-OMe;IO166D Gold 12 nm PEG-OMe
NP00478			Au_PEG-OH/PEG-OMe(50:50)

Add | Close

Confirm Input for **Analysis-0000000046**

NanoParticles Input	1 NanoParticle selected: NP00809 Selected number of NanoParticles OK
Protein Input	2 Proteins selected: P06276 Q9BV73 Please select exactly one Protein

Adjust Input

Integrated Services – Corona model

NanoCommons
Nano-Knowledge Community

Nanoparticle
NP00477

NanoParticle	NP00477
Names	Au_PEG-OH;IO166B Gold 12 nm PEG-OH
Description	

Protein
Q9GU57

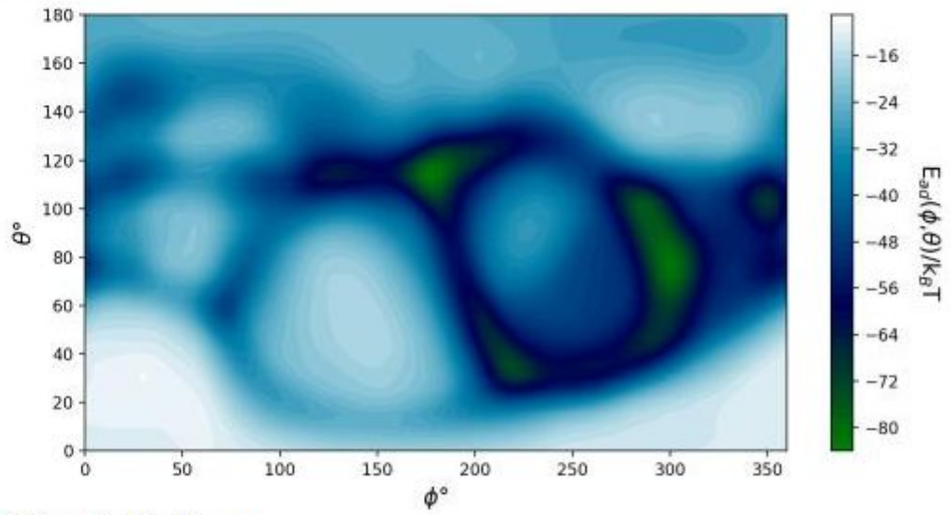
Protein	Q9GU57
ProteinName	Conotoxin Gm9.1

PDB Structure
1IXT

PDB ID	1IXT
Description	structure of a novel p-superfamily spasmodic conotoxin reveals an inhibitory cystine knot motif

Size & Zeta Potential

Size [nm]: 12.0
Zeta Potential [mV]:16.7



Mapping: 1IXT_gold_12_16.map
LogFile: Analysis-0000000098.log

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Next steps -

API based integrations

- eNanoMapper/AMBIT
- ACEnano
- NECID
- EUON
- Modelling and Analysis tools

Date integration

- Modelling results
- TAs

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Partnerships

- **Application projects**
  More than 20 Biomax customers have over 1000 end-users

- **Research projects**
  Biomax technology is used in over European and international researc projects with well ove

European Patent Office

info@biomax.com - www.biomax.com

Thank you!

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