



**NanoCommons**

Nano-Knowledge Community

**NanoCommons Knowledge Base**  
***Data services used in successful TAs***

**dieter.maier@biomax.com**

***SbD Workshop***  
***9th November 2021***

# Successful data TAs

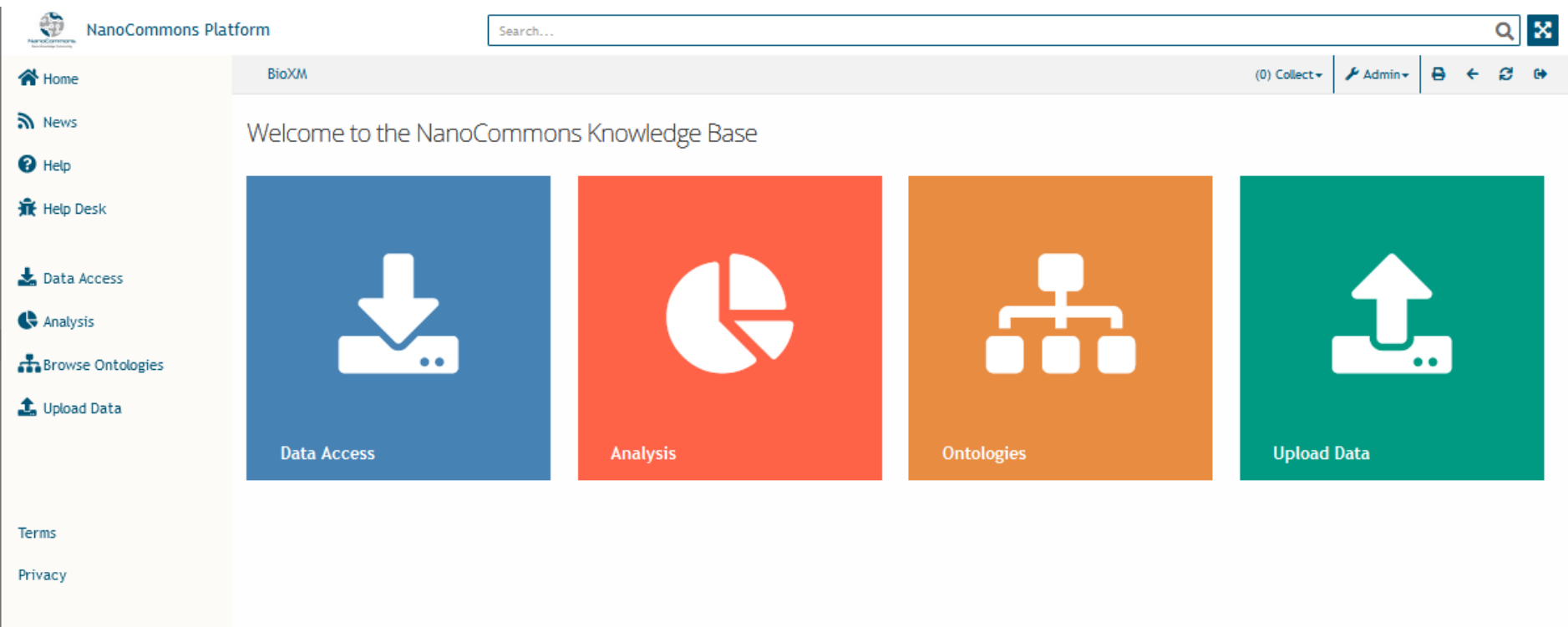
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- **NanoFASE - complex EcoTox data**
- **SmartNanoTox - real and computational NM characterisations**
- **UCD/PLUS - validation of protein corona prediction**

# Data services in the NanoCommons Knowledge Base

<https://ssl.biomax.de/nanocommons/>

**Please autoregister on the login page to get access**



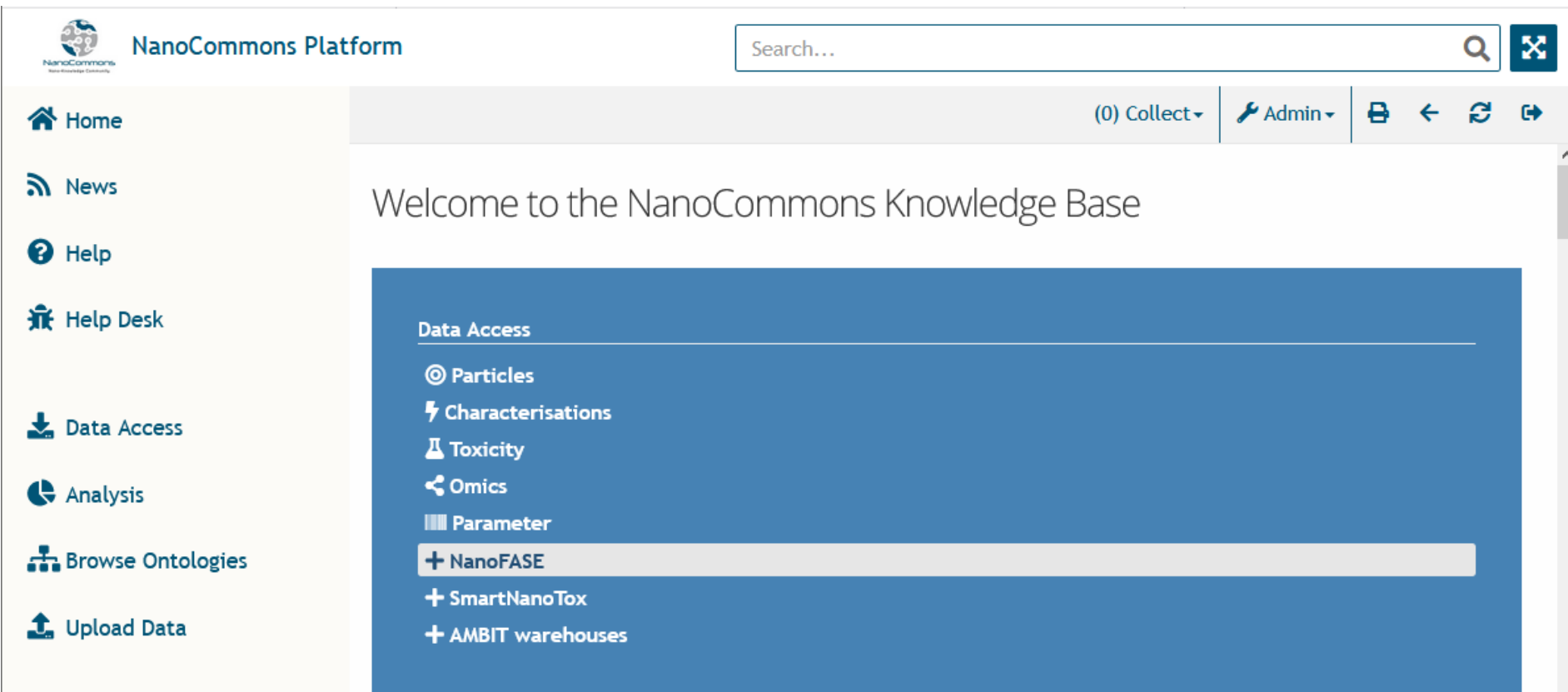
The screenshot displays the NanoCommons Platform interface. At the top left, the NanoCommons logo and the text "NanoCommons Platform" are visible. A search bar is located at the top center. The main content area is titled "BioXM" and includes a navigation menu on the left with items: Home, News, Help, Help Desk, Data Access, Analysis, Browse Ontologies, and Upload Data. The main content area features a welcome message "Welcome to the NanoCommons Knowledge Base" and four large, colorful buttons: "Data Access" (blue), "Analysis" (orange), "Ontologies" (light orange), and "Upload Data" (teal). Each button contains a white icon representing its function. The bottom of the page shows "Terms" and "Privacy" links.

# NanoFASE - complex EcoTox data

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- complex template (NIKC), representing multiple measurements for each "instance" along ecological NM life-cycle
- detailed protocols given
- multiple groups involved with individual data sets
  - => standard template required
  - => adapted NIKC template to NanoFASE requirements (UoB, Tassos)
  - => data shepherding required to fill template (UoB, Tassos)
  - => data upload service required (Biomax, Beatrix)

# Result - Full integration



The screenshot displays the NanoCommons Platform interface. At the top left is the NanoCommons logo and the text "NanoCommons Platform". To the right is a search bar with the placeholder text "Search...". Below the search bar is a navigation bar with the following elements: "(0) Collect", "Admin", and a set of navigation icons (back, forward, refresh, home). On the left side, there is a vertical menu with the following items: Home, News, Help, Help Desk, Data Access, Analysis, Browse Ontologies, and Upload Data. The main content area features a large blue box with the text "Welcome to the NanoCommons Knowledge Base". Below this text is a list of categories under the heading "Data Access": Particles, Characterisations, Toxicity, Omics, Parameter, NanoFASE, SmartNanoTox, and AMBIT warehouses. The "NanoFASE" item is highlighted with a light gray background.

# Data can be embargoed as required

## NanoFASE

NanoFASE data is embargoed until 9/2021. For earlier access please agree and exchange a [data analysis agreement](#) with the corresponding data owner.

Initial contact for requests of NanoFASE data is Lee Walker [leew@ceh.ac.uk](mailto:leew@ceh.ac.uk) at the project coordinating institution [UK Centre for Ecology and Hydrogeology](#)

NanoFASE publicly available information: List of measured parameters

< 1 of 3 > Per page: 25 Results: 71

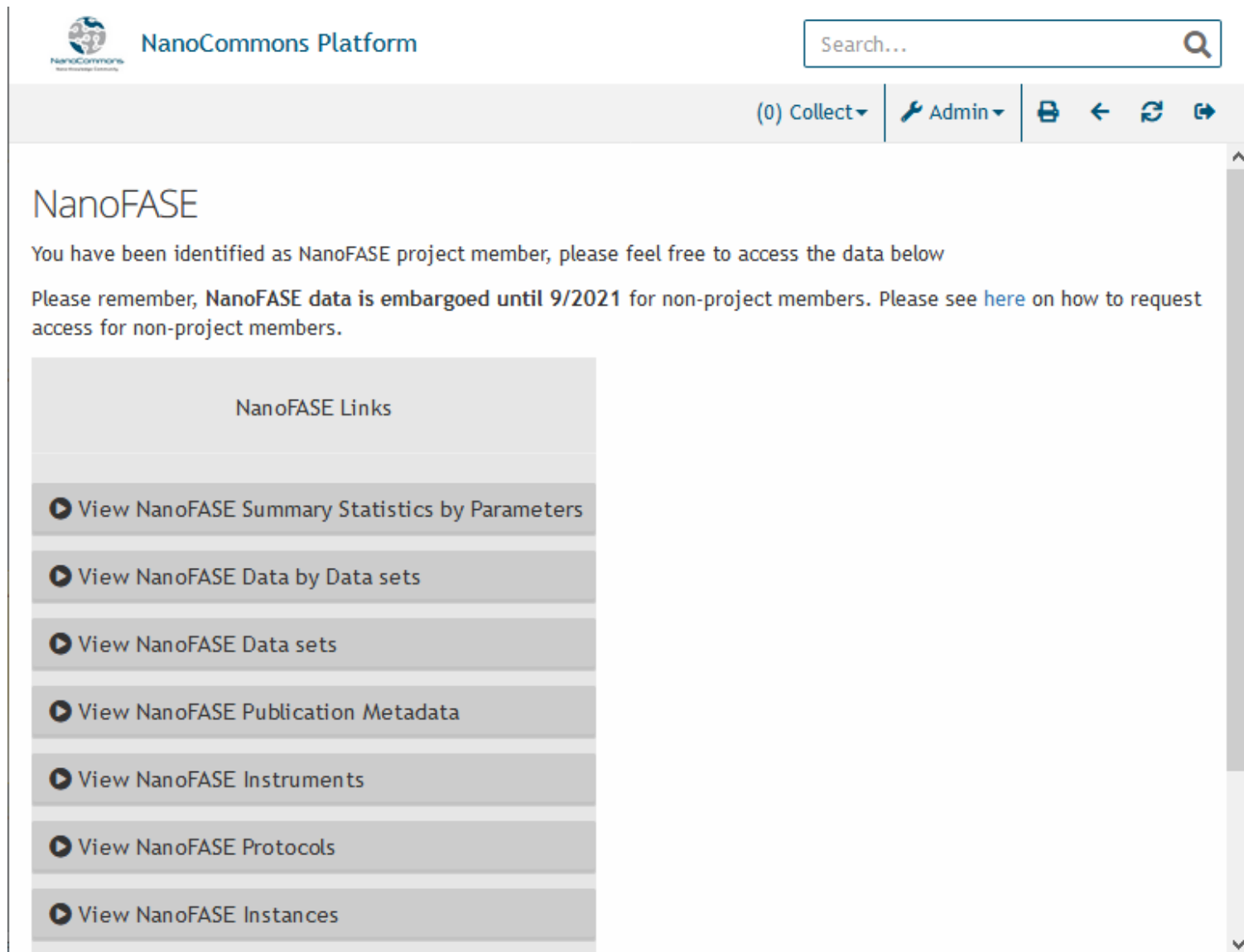
Filter results by:

Selected items: 0

Show/Hide ▾ Sorted by Parameter ▾

Parameter	Ontology mapping	Parameter Synonyms	Description	Data type
<input type="checkbox"/> Ag presence determination		Ag presence determination		
<input type="checkbox"/> Ag2S concentration				numeric
<input type="checkbox"/> AgNO3 concentration				numeric
<input type="checkbox"/> AgNPs concentration				numeric

# Overview on NanoFASE data



The screenshot displays the NanoCommons Platform interface. At the top left is the NanoCommons logo and the text "NanoCommons Platform". To the right is a search bar with the placeholder text "Search...". Below the search bar is a navigation bar with the following elements: "(0) Collect", "Admin", and several utility icons (print, back, refresh, forward). The main content area is titled "NanoFASE" and contains the following text:

You have been identified as NanoFASE project member, please feel free to access the data below

Please remember, **NanoFASE data is embargoed until 9/2021** for non-project members. Please see [here](#) on how to request access for non-project members.

Below the text is a section titled "NanoFASE Links" which contains a list of seven links, each with a play button icon:

- ▶ View NanoFASE Summary Statistics by Parameters
- ▶ View NanoFASE Data by Data sets
- ▶ View NanoFASE Data sets
- ▶ View NanoFASE Publication Metadata
- ▶ View NanoFASE Instruments
- ▶ View NanoFASE Protocols
- ▶ View NanoFASE Instances

# NanoFASE Protocols







## NanoFASE Protocols

< 1 of 2 > Per page: 25 Results: 38

Filter results by:

Selected items: 0

Show/Hide ▾ Sorted by Protocol Name ▾

Protocol Name	ID	Description	Step ID	Step Name	Step Description	Step Duration value	Step Duration unit	Instances
<input type="checkbox"/> Acid digestion of animal tissues	 DS00000606_1		1.0	sample freeze	dry powder	250.0	uL	
			2.0	dried	tubes carefully cleaned	40.0	min	IN000012784
			3.0	sample weighed	85° C	40.0	min	
			4.0	into digestion tube	130° C	60.0	min	IN000012785
			5.0	on microbalance	160° C		till	
			6.0	add 7:1 mixture of	180° C		dryness	IN000012786
			7.0	HNO3 (65% (Baker				
			8.0	Ultrax II Ultra				IN000012795
			9.0	Pure)) and HClO4 (70% (Baker Ultrax				 IN000012796



# NanoFASE Instruments

## NanoFASE Instruments

< 1 of 2 > Per page: 25 Results: 35

Filter results by:











Model

Apply

+ Add Filter

Selected items: 0

Show/Hide  Sort by

			Manufacturer	
Model	Instrument Name	Name	Country	
<input type="checkbox"/>  JEM-2100	HR-TEM	 JEOL	United Kingdom	
<input type="checkbox"/>  D5000	XRD	 Bruker		
<input type="checkbox"/>  Agilent 7500	ICP-MS	 Agilent Technologies	USA	
<input type="checkbox"/>  CEM 1600W	Analytical microwave digestion system	 MARS		
<input type="checkbox"/>  NR50 E	end-over-end shaker	 OVAN		

# SmartNanoTox - real and computational NMs

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- combining real and computational NMs with experimental determined and computational predicted properties
- all data collected by coordinator (allows single batch upload)
  - => data warehouse upload adapted to SNT template (Biomax)
  - => data upload service called for (Biomax)

# SmartNanoTox data

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## Access to SmartNanoTox data

SmartNanoTox has selected the NanoCommons Knowledge Base to make available its extensive data on computational material property and protein corona predictions.

SmartNanoTox results are available under the [Creative Commons Attribution 4.0 License](#). You are therefore allowed to freely use the data as long as you cite the originator. Please include the following reference whenever citing SmartNanoTox data:

### SmartNanoTox Links

- ▶ [View SmartNanoTox Nanomaterials](#)
- ▶ [View SmartNanoTox Parameters](#)
- ▶ [View SmartNanoTox Corona predictions](#)

# 170 NMs with Shape, Zeta, TEM

All SmartNanoTox Particles (real and computational)

< 1 of 7 > Per page: 25 Results: 170

Filter results by:







Apply

+ Add Filter












Selected items: 0

Show/Hide

Sorted by ID

Usage conditions							Further Information		
ID	License	Reference	Chemical Elements	Characterisation data	Samples	Aliquots	All names	Description	Aging reaction
<input type="checkbox"/>  NP01175	Released under Creative Commons 4.0 license (use freely as long as you cite)		 Ti	 Computational-TiO2-Anatase101.01			Computational-TiO2-Anatase101.01, Anatase101, TiO2-anatase	Uncoated	
<input type="checkbox"/>  NP01176	Released under Creative Commons 4.0 license (use freely as long as you cite)		 Ti	 Computational-TiO2-Anatase101.02			Computational-TiO2-Anatase101.02, Anatase101, TiO2-anatase	Uncoated	

# Adsorption energy predictions

ID	Chemical Element	Names	Description	CHEBI entry	Relations (Adsorption)	
					Target	Adsorption Energy
<input type="checkbox"/>	 NP01175	 Ti	Computational-TiO2-Anatase101.01, Anatase101 TiO2-anatase	Uncoated	 P35247	-25.69585221
					 O00206	-52.368073
					 P02787	-56.66557289
					 P61626	-41.34195176
					 P01308	-23.13611604
					 P02768	-67.52882332
					 P01861	-41.12133827
					 P15782	-23.31471318
					 P15785	-2.282227441
					<input type="checkbox"/> CHEBI:16113 cholesterol	0.671485724
					<input type="checkbox"/> CHEBI:18295 histamine	0.49947338
					<input type="checkbox"/> CHEBI:18237 glutamic acid	-6.5437572
					<input type="checkbox"/> CHEBI:15428 glycine	0.16088794
					<input type="checkbox"/> CHEBI:16449 alanine	0.9590677
					<input type="checkbox"/> CHEBI:25017 leucine	1.09745976
					<input type="checkbox"/> CHEBI:29016 arginine	-0.96450462
					<input type="checkbox"/> CHEBI:27897 tryptophan	0.63699254
					<input type="checkbox"/> CHEBI:26271 proline	0.43076368
					<input type="checkbox"/> CHEBI:26986 threonine	0.7329866
					<input type="checkbox"/> CHEBI:27266 valine	1.02156734
					<input type="checkbox"/> CHEBI:17822 serine	0.70440536

# UCD/PLUS - validate protein corona prediction

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- complex workflow combining image analysis, computational prediction - comparative experimental evidence
- Phys-Chem data covered by standard NC KB template
- Bioassay (protein binding) data covered by standard NC KB "Experimental data" template

=> usability adaptations required for upload (PLUS, Biomax)

- UI clarification + simplification
- Online help extended

=> application integration into NC KB (UCD, NovaM, Biomax)

- NanoXtract image analysis tool
- Corona prediction model

# Comparing prediction and experiment

## Corona Analysis Overview

+ New Analysis Run

☰ Task Manager

Per page: 25 Results: 9




































Filter results by:

Analysis ID















Apply

+ Add Filter

Show/Hide Sort by

Analysis ID	NanoParticle ID	Protein ID	Analysis Start	Started by User	Analysis Results	
					Heatmap	Mapping
 Analysis-000000098	 NP00477	 Q9GU57	Feb 19, 2020 1:49:22 PM	 martinz		1IXT_gold_12_16.map
 Analysis-000000102	 NP00728	 P04264	Feb 21, 2020 6:17:13 PM	 dm_admin		6E2J_tio2_anatase_25_12.map
 Analysis-000000107	 NP00478	 Q16696	Feb 24, 2020 9:46:18 AM	 martinz		3T3S_sio2_amorphious_12_-8.map
 Analysis-000000202	 NP00477	 Q9AHD4	Feb 28, 2020 10:20:48 AM	 martinz		3QY8_gold_12_16.map
 Analysis-000000710	 NP00476	 P04063	Mar 31, 2021 11:37:11 AM	 martinz		1BG9_gold_12_-16.map
 Analysis-000000704	 NP00728	 P04264	Mar 24, 2021 4:27:11 PM	 dm_admin		6E2J_tio2_anatase_25_12.map
 Analysis-000000505	 NP01113	 P15494	Jan 15, 2021 10:19:47 AM	 ingridhasenkopf		4A88_sio2_amorphious_114_-23.map

# Adsorption energy predictions

Assay (NP01113-P15494_4)	
Assay	 NP01113-P15494_4
Name	NP01113-P15494_4
Method	 Other assay
Format	Values
Number of endpoints	6
Description	
Protocol file	 MetadataNP-ProteinBinding_BCA.pdf  MetadataNP-ProteinBinding_BCA.pdf  MetadataNP-ProteinBinding_SDS.pdf  NP01113 Metadata PTMO+Bet ChemiDoc.xlsx
Raw data	 PTMOSiO2+Betv1.Gel.png
Creation time	07.04.2021 17:29:36
Assay (NP01113-P15494_7)	
Assay	 NP01113-P15494_7
Name	NP01113-P15494_7
Method	 Other assay
Format	Values
Number of endpoints	6
Description	
Protocol file	 MetadataNP-ProteinBinding_BCA.pdf  MetadataNP-ProteinBinding_BCA.pdf  MetadataNP-ProteinBinding_SDS.pdf  NP01113 Metadata PTMO+Bet ChemiDoc.xlsx
Raw data	 PTMOSiO2+Betv1.Gel.png
Creation time	07.04.2021 17:29:36



## Summary - Data services

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- Cooperatively develop templates for data collection
- Data collection/curation shepherding
- Adapt data upload to project template
- Provided upload user interface and online help/tutorial
- Data upload services
- FAIRification
- Integration with existing data warehouses (e.g. AMBIT)

### 1. NC KB data retrieval integrating

- NC KB data warehouse (NanoMILE, NanoFASE, NanoGen, NanoSolveIT, SmartNanoTox, TA data)
- AMBIT hosted data (eNanoMapper, NanoReg, NanoReg2)

=> 1506 NMs total (604 NC KB, 902 AMBIT)

=> 500 parameters (452 NC KB, 48 AMBIT)

=> >8000 PhysChem and Tox datasets

### 2. NanoXtract Image analysis tool + Protein corona prediction (if time allows)