SmartNanoTox
Smart Tools for Gauging Nano Hazards

Data strategy and relevance for Nanoinformatics and Nanosafety projects

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SmartNanoTox
Smart Tools for Gauging Nano Hazards
Horizon 2020
European Union funding
for Research & Innovation

Project legacy

Concepts

- Mechanism-based toxicity assessment paradigm

PATROLS
Advanced Tools for NanoSafety Testing

Methods and SOPs

- NM labelling, tracking, post-uptake characterisation
- ALI exposure imitation, aerosolisation, exposure quantification
- Bionano interaction modelling
- Pathway analysis, GRN analysis, omics data processing

OECD
WPMN

NanoSolveIT

Models

- QSARs for MIE/KE
- Protein adsorption and corona models

NanoCommons
Nano-Knowledge Community

Data

- In vivo: histology, omics, AOPs, GRNs, AOPs, MIEs, KEs
- In vitro: cell culture tox assays, NM tracking, NM corona, ROS, surface tension
- In silico: NM properties, bionano interactions

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SmartNanoTox outcomes: Toxicology

- Description of 5 respiratory AOPs, identified KE/MIE, tools for KE/MIE – **AOP Wiki, NanoCommons**
- Gene expression profiles for *in vivo* respiratory exposure – **GEO database**
- Novel ALI systems to imitate realistic exposure conditions - **Vitrocell**
- Novel analysis protocols for inference of GRNs from transcriptomics data, identification of Core Regulatory Genes – **NanoCommons**

Gene Expression Omnibus

VITROCELL SYSTEMS

Available via project website www.smartnanotox.eu

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Project outcomes: Nanoparticles

- Novel NM labelling techniques – **JSI, SNT website**
- Novel protocols for corona analysis – **SNT website**
- Novel algorithms for image analysis / colocalization – **JSI**
- Protein corona-based NM fingerprints – **NanoCommons KB**
- NM tracking techniques, post-uptake characterisation data - **JSI**
- Atomistic, coarse-grained force fields for common materials (30 materials) – **NanoSolveIT**, **OpenKIM**, **SNT website**
- Multiscale simulation tools for bionano-interface – **NanoCommons KB**
- Novel advanced NM and protein descriptors (over 30 new descriptors, 60 materials) – **NanoCommons KB**
- Publicly available database of bionano interactions – **NanoCommons KB**

Project outcomes: Industry/Regulation

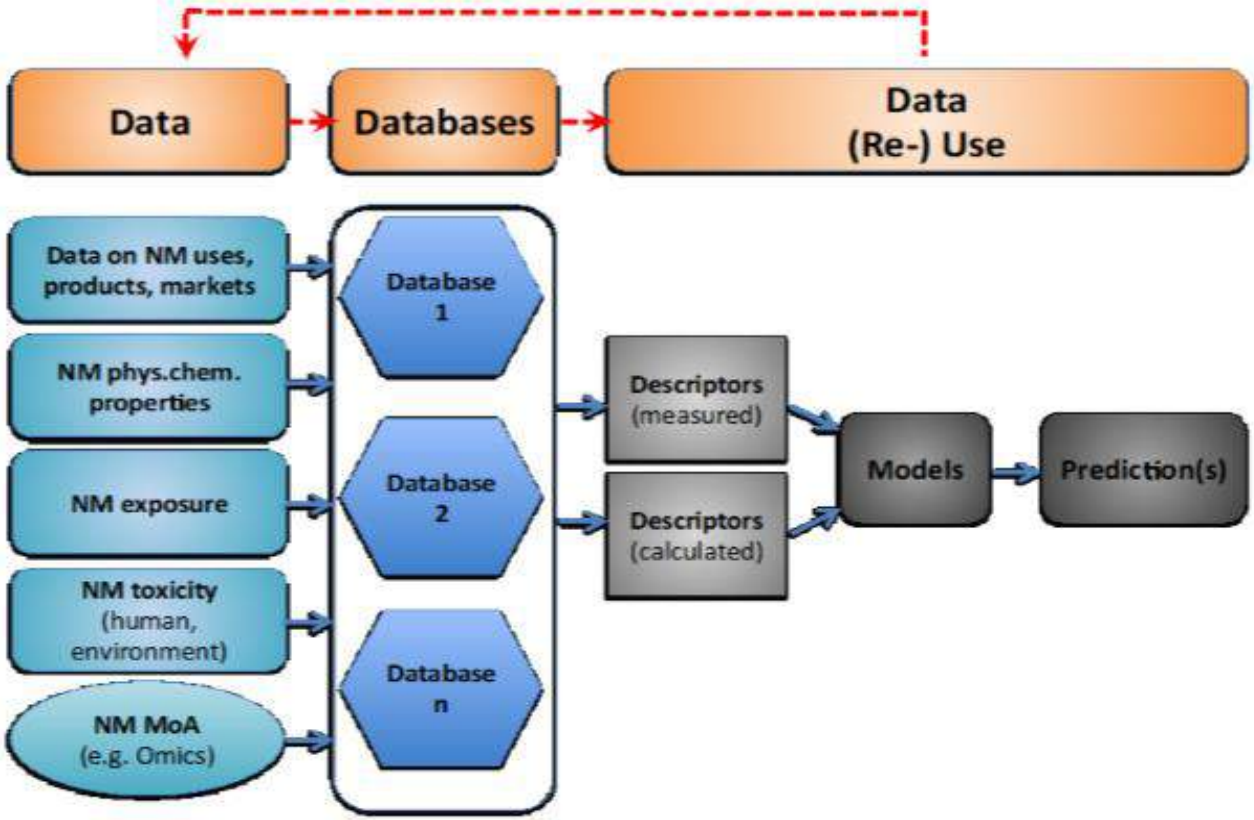
- Novel toxicity endpoints bound to in vivo AOPs
- Novel in vitro assays targeting MIE/KE based on reporter gene
- Elucidation of toxicity mechanisms for oxides, carbonaceous materials
- Creation of basis for read-across and safety by design through identification of NM properties of concern
- Mechanism-aware QSARs relating NM properties to biological activity – **SNT Website**

SmartNanoTox materials

- Titania (TiO_2): 16 NMs – rutile, anatase, spheres, tubes
- Quartz and Silica: 3 NMs
- Metal oxides: 7 NMs Fe_2O_3, ZnO, $Ni_xFe_yZn_zO_u$
- Carbon black: 2 NMs
- Carbon nanotubes: 28 SWCNTs and MWCNTs
- Graphene: 3 NMs
- Asbestos: Crocidolite

Nanoinformatics

Relevant NM characterisation data are necessary to build predictive models



https://www.nanosafetycluster.eu/Nanoinformatics2030.html

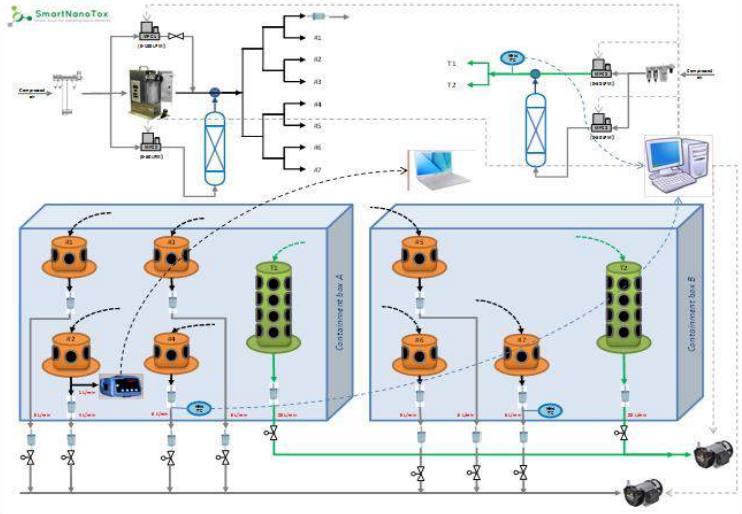
Contribution to nanoinformatics

- NM properties measured/calculated for many NMs
- Novel NM descriptors: bionano interface, surface activity
- Methods of in silico NM characterisation: ab initio multiscale models
- Mechanism-aware QSARs relating NM properties to biological activity MIE/KE
- Grouping of materials based on their bio-relevant activities

SmartNanoTox Data: in vivo

- Inhalation: rats, mice
- Instillation: mice
- 3 time points
- 3 concentrations
- 15+ NMs

A



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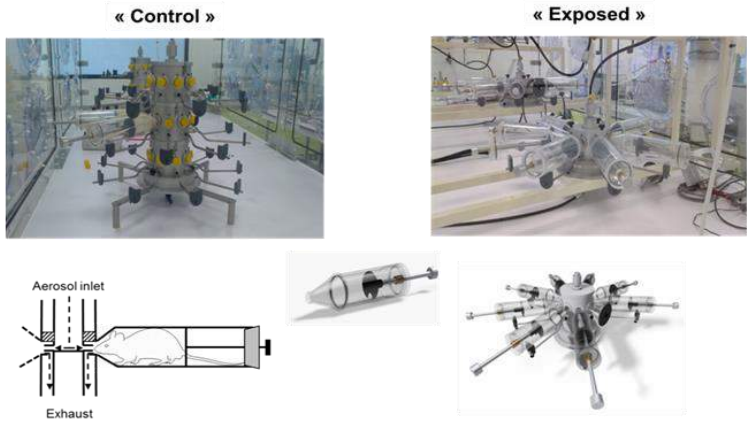

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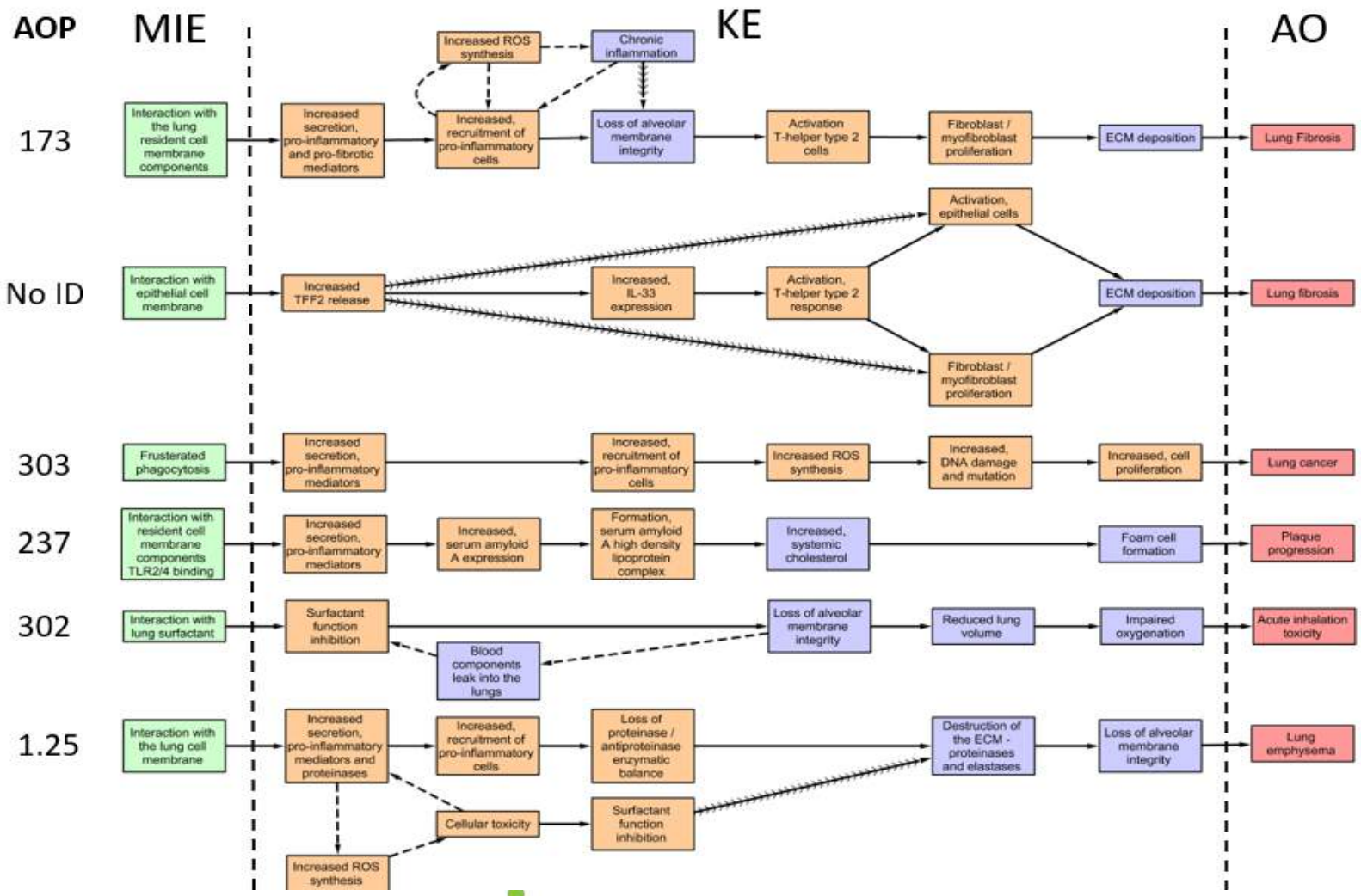
SmartNanoTox Data: in vivo

Study	Activity	Activity Description	Type of data for sharing	Shared Format	Archive
NMs / Tissues	'Omics	Studies for in vivo reaction to inhalation/ instillation of NMs: gene expression, metabolomics, proteomics	Candidate Gene and Protein IDs	MaxQuant Data CSV*	PRIDE, GEO, Zenodo
Inhalation / IT instillation of NMs	In vivo tox tests in mice	Inhalation experiments: defined NMs aerosolisation, & investigation of interactions of NM within the lung lining fluid, alveolar epithelial cells & macrophages	Toxicological endpoints - Tissue for histological evaluation and gene profiling, analysis of biological endpoints	data sheets, CSV*	SNT, Zenodo
Lung-specific or respiratory AOP	Toxicity Pathway Identification	Identify pathways for lung diseases from GEO & biological processes perturbed by NM uptake	Candidate Pathways	CSV*	GEO, Zenodo
IT instillation of NMs	In vivo tox tests in mice	Instillation experiments: Investigation of interactions of NM within the lung lining fluid, alveolar epithelial cells and macrophages	Toxicological endpoints/Tissue for histological evaluation & gene profiling, analysis of biological endpoints	CSV*	Zenodo
Lung tissue	Histology evaluation	Tissue analysis of in vivo samples	**Verbal** evaluation, Semi-quantitative scores	CSV*, images**, MDs	SNT, Zenodo

Network of NM-induced AOPs

Figure 1



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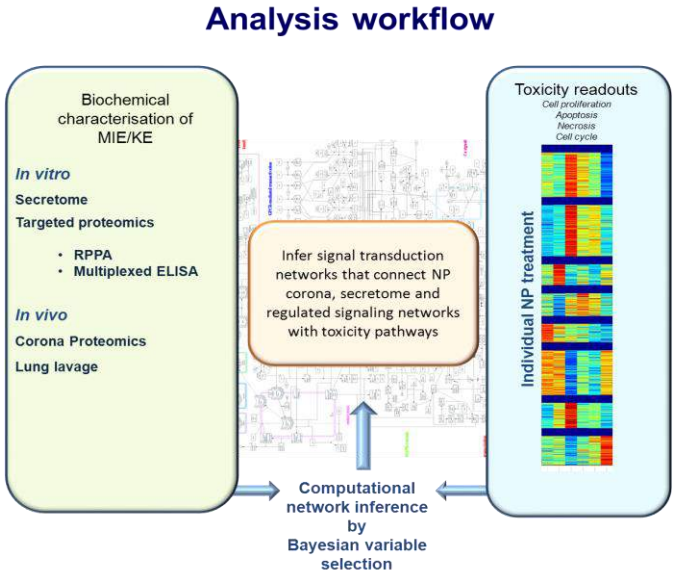
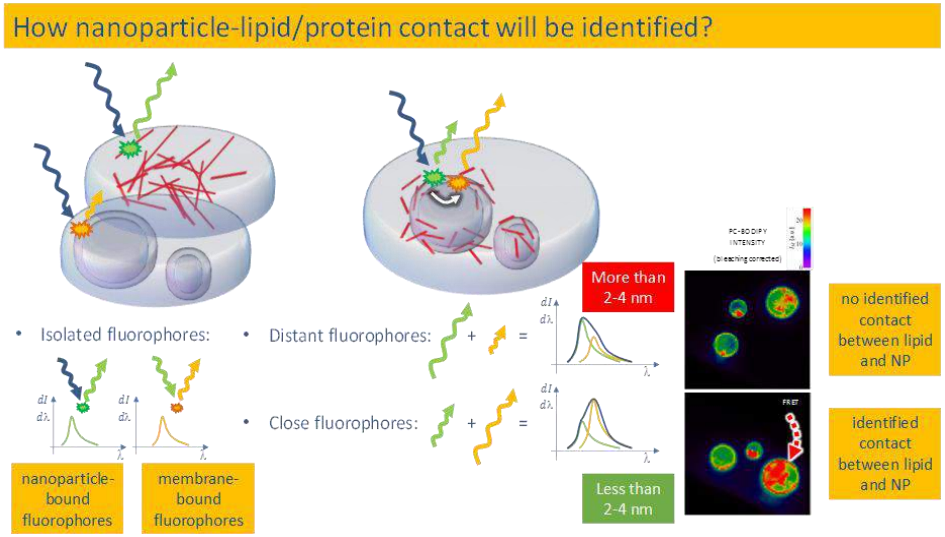
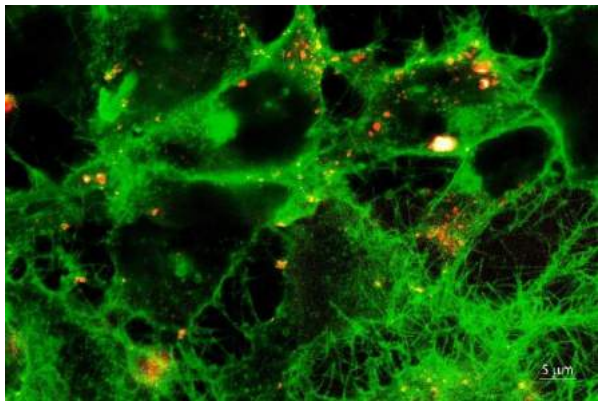
SmartNanoTox Data: in vitro







SmartNanoTox Data: in vitro

Study	Activity	Activity Description	Type of data for sharing	Shared Format	Archive
NMs	Lipidomics	Content & evolution of the NM biomolecular corona & lipid wrap/NM containing complexes from in vivo exp.	MS derived Lipid IDs	Spectral Data CSV*	SNT, Zenodo
Lung cells	In vitro tox tests in murine cells	Cell-line exposure experiments using Vitrocell exposure systems	Cytotoxicity and biological endpoints (gene-/protein-level)	data sheets, CSV*	SNT, Zenodo
NMs	Surface Tension Experiments	Investigation of NM interaction with the lung alveolar fluid and lung integrity	Surface tension profiles, dose-response curves Effect of NMs on lung surfactant surface tension, inhibitory dose	CSV*	Zenodo
Labelled NPs	FMS	NM modification for efficient tracking (fluorescent/isotopic labelling)	fluorescence spectra - procedures for labelling nanoparticles & characterize the efficiency of labelling	spectra, synthetic pathways, CSV*	LBF Website, Zenodo
Labelled NPs / cell lines	FMS, 3D STED spectral data	NM modification for efficient tracking (fluorescent/isotopic labelling)	2D & 3D stack of 2D images (4D & 5D sets of data) - images, evaluation of affinity constants, lifetimes of states, characteristic times of membrane changes	Images**, text data*, Video	LBF Website, Zenodo
NPs / BALF / Lipid dispersion	In vitro 'NP' to lipid affinity	Analysis of NM-lipid interaction for labelled NMs	autocorrelation curves analysis & stack of images - images, evaluation of affinity constants	Text data, CSV*, Images**	LBF Website, Zenodo
Lung cells	In vitro tox tests rat & human cells	Analysis of cell responses to NMs	Cytotoxicity and biological endpoints (gene-/protein-level), included transcriptomics	data sheets CSV*	SNT, Zenodo

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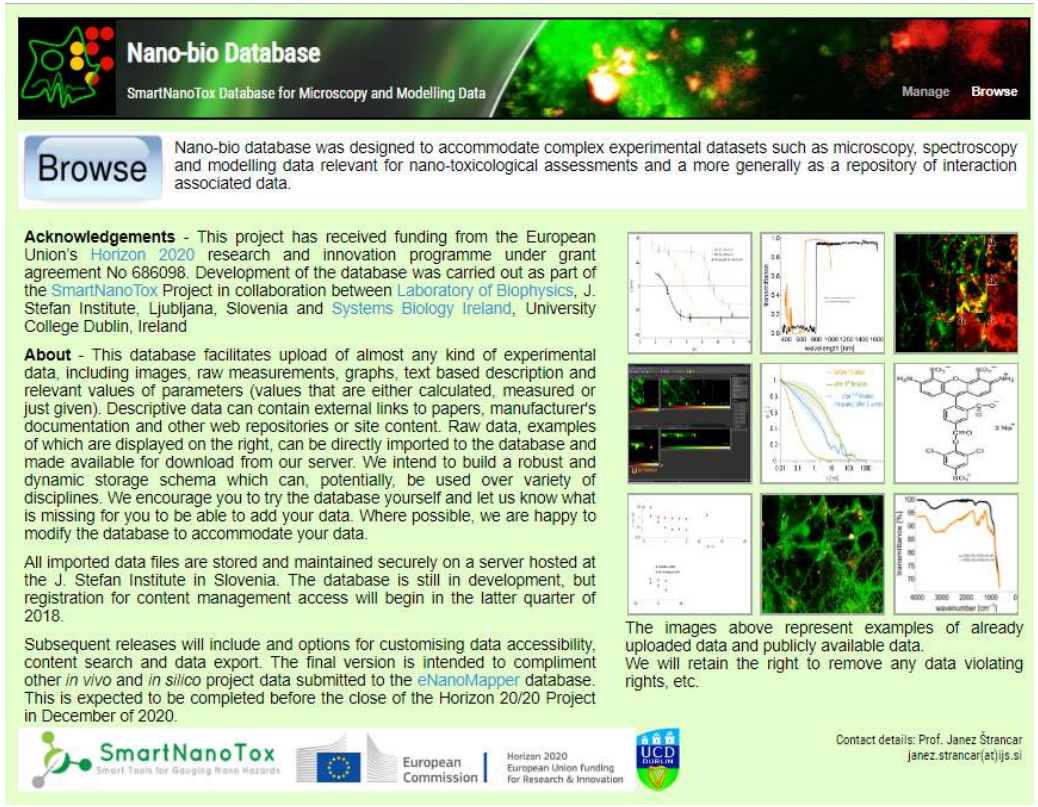
LBF XML Data Schema

Underlying Schema

- Comprehensive set of XML tags for describing location, image, text & numerical data.
- XML paired with styling info. should render in any browser if/when downloaded.

Data Service

- Current version (public) lbfnanobiodatabase.ijs.si.
- Components can be referred to explicitly or searched via URI.



- An unreleased version facilitates data search and personalised user 'libraries'.
- Libraries can be shared between users (service) or made public &| downloadable.

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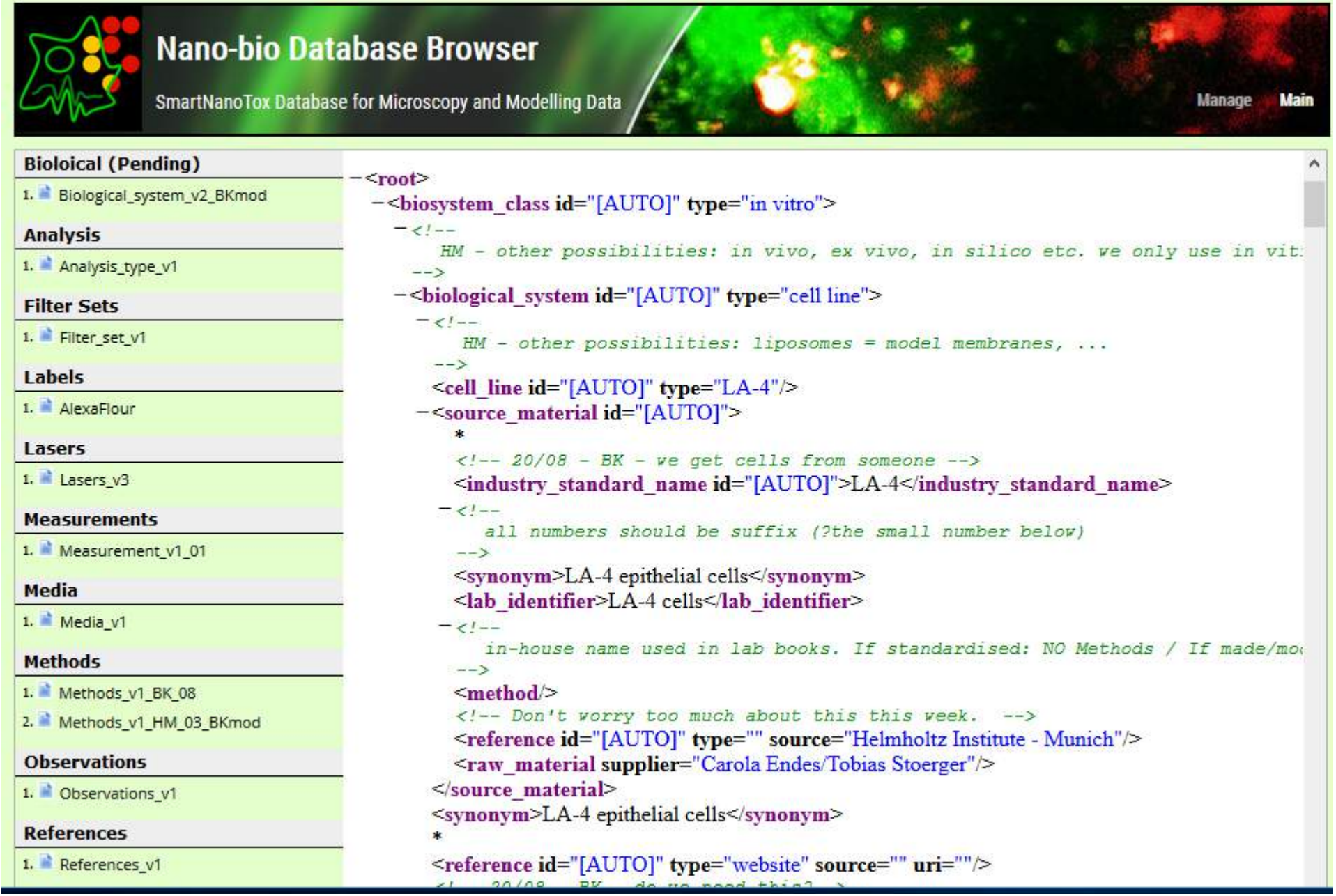
Nano-bio Database Browser
SmartNanoTox Database for Microscopy and Modelling Data
Manage
Main
Bioloical (Pending)
1. Biological_system_v2_BKmod
Analysis
1. Analysis_type_v1
Filter Sets
1. Filter_set_v1
Labels
1. AlexaFlour
Lasers
1. Lasers_v3
Measurements
1. Measurement_v1_01
Media
1. Media_v1
Methods
1. Methods_v1_BK_08
2. Methods_v1_HM_03_BKmod
Observations
1. Observations_v1
References
1. References_v1
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HM - other possibilities: in vivo, ex vivo, in silico etc. we only use in vit
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HM - other possibilities: liposomes = model membranes, ...
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*
20/08 - BK - we get cells from someone
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in-house name used in lab books. If standardised: NO Methods / If made/mo
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Don't worry too much about this this week.
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Nano-bio Database Browser

SmartNanoTox Database for Microscopy and Modelling Data

Manage Main

Bioloical (Pending)

1. Biological_system_v2_BKmod

Analysis

1. Analysis_type_v1

Filter Sets

1. Filter_set_v1

Labels

1. AlexaFlour

Lasers

1. Lasers_v3

Measurements

1. Measurement_v1_01

Media

1. Media_v1

Methods

1. Methods_v1_BK_08
2. Methods_v1_HM_03_BKmod

Observations

1. Observations_v1

References

1. References_v1

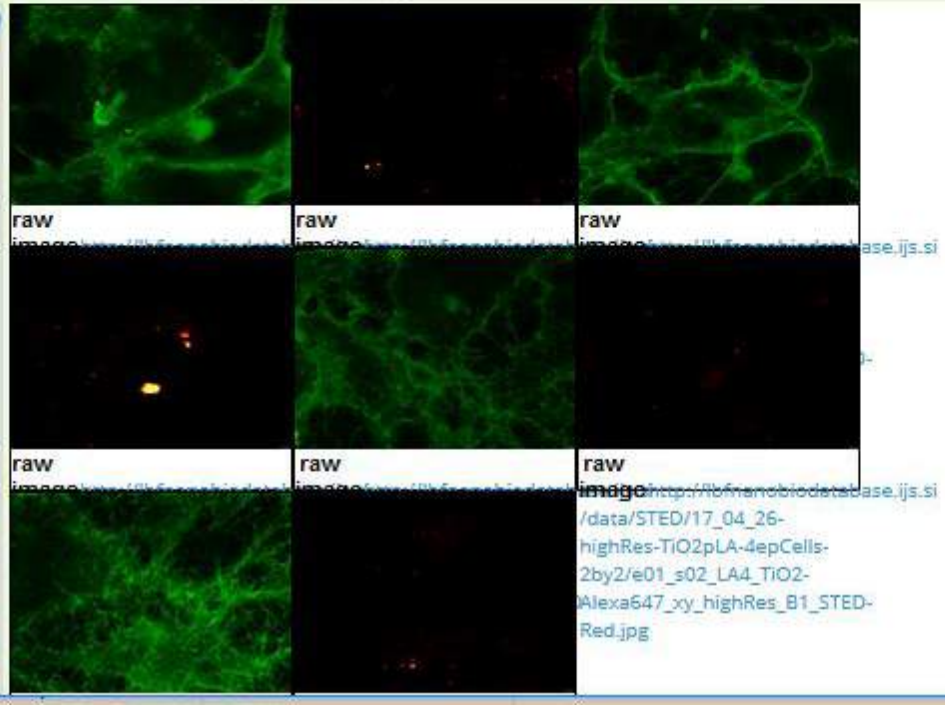
Method Class Optical microscopy

ID:[AUTO] Method STED microscopy

Observation(s)

Type	co-localization [Parent: microscopy imaging]
Desc	TiO2 nanotubes are co-localizatied within LA-4 epithelia cell membrane. Conclusion is based on overlay of red and green channel signal.
Type	membrane disruption [Parent: microscopy imaging]
Desc	TiO2 disrupts LA-4 epithelia cell membrane. Not sure about this one. We have to be careful to only state here what is realy seen from an image
Type	membrane wrapping [Parent: microscopy imaging]
Desc	TiO2 wraps into LA-4 cell membrane building blocks . Conclusion is based on overlay of red and green channel signal.

Raw Data (Images)



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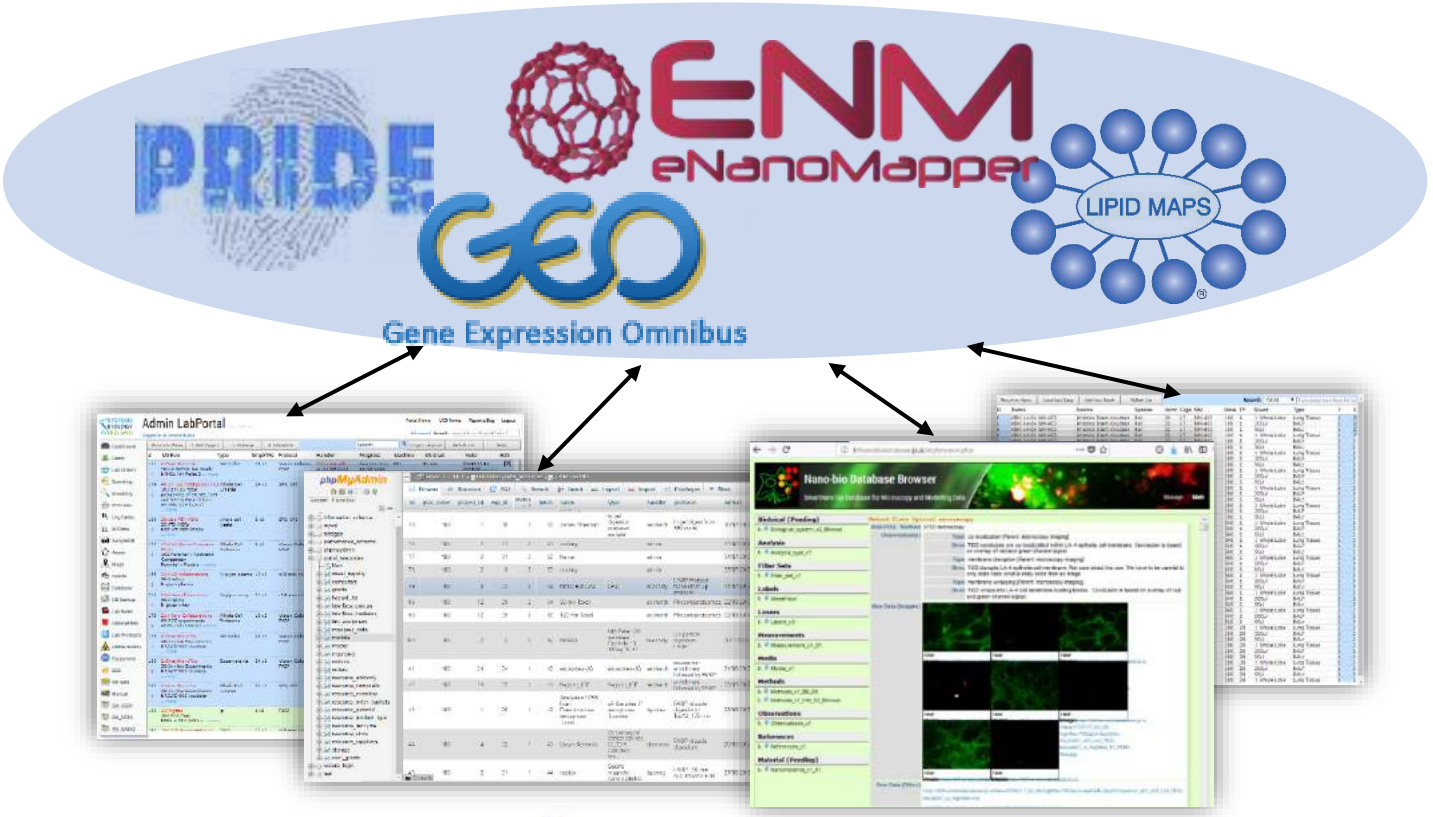
Development of Novel Data Services

- SNT data which is not eNM/NC KB compliant and lack an established or centralised data repository can be transformed into XML databases and referenced via embedded URIs.



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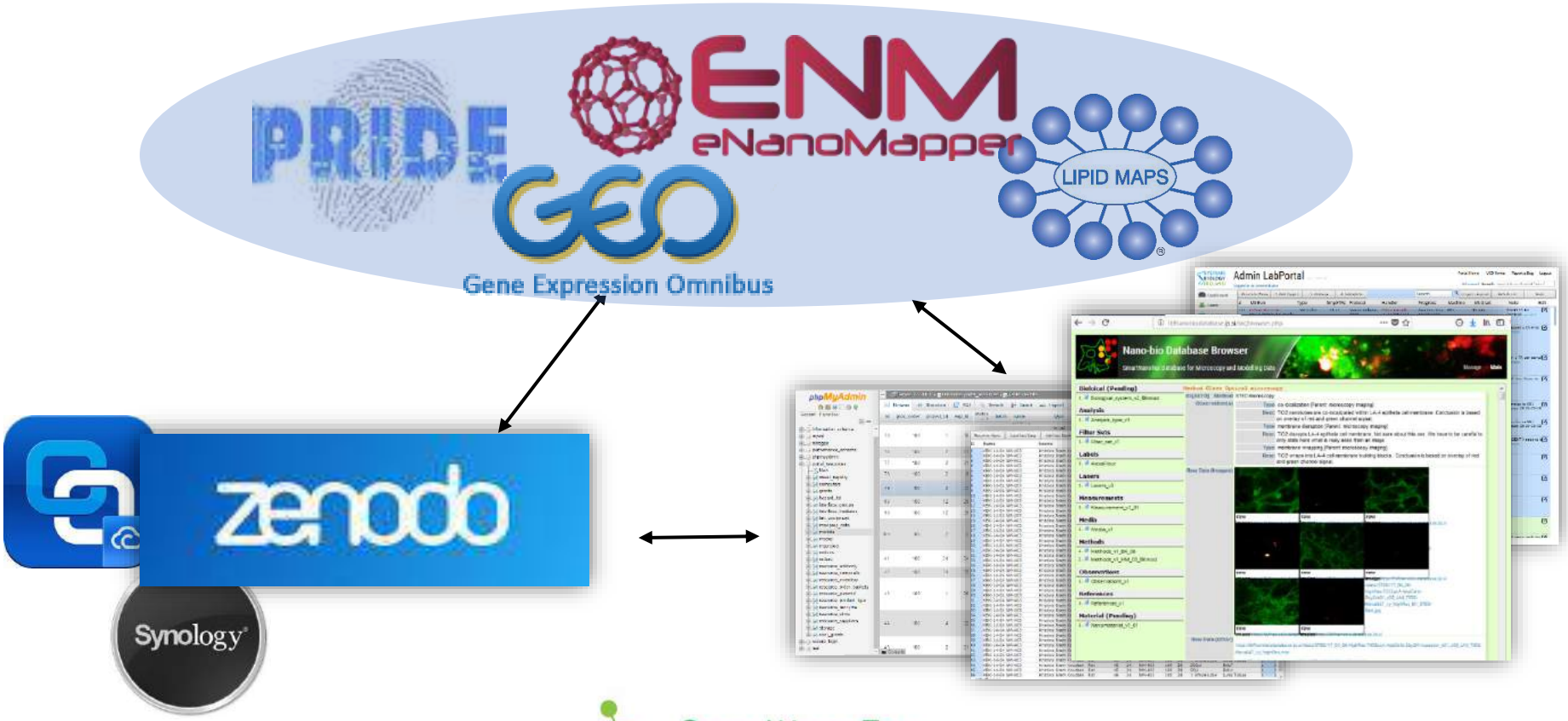
Supplementary File Storage

- 200+ GB Simulation data and 2+ TB Proteomics not all shared via research repositories.
- Large volume data storage will be hosted via NAS & Zenodo File storage services.



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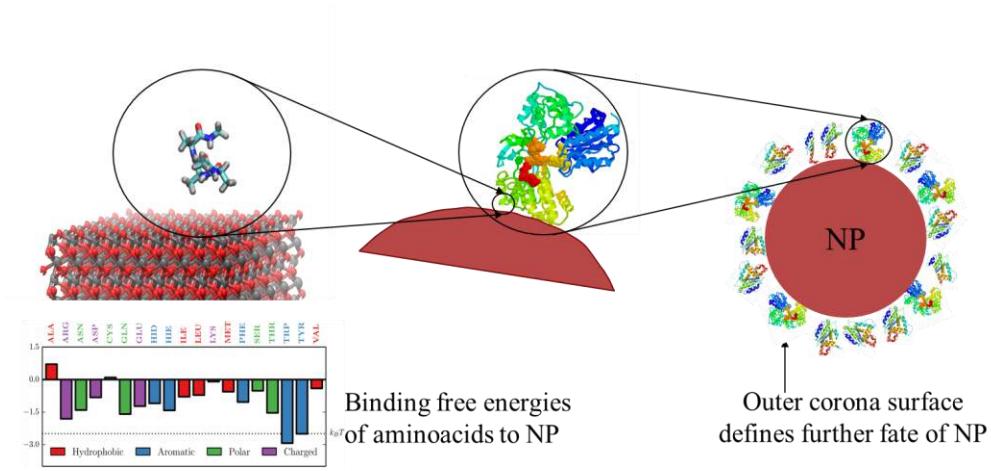
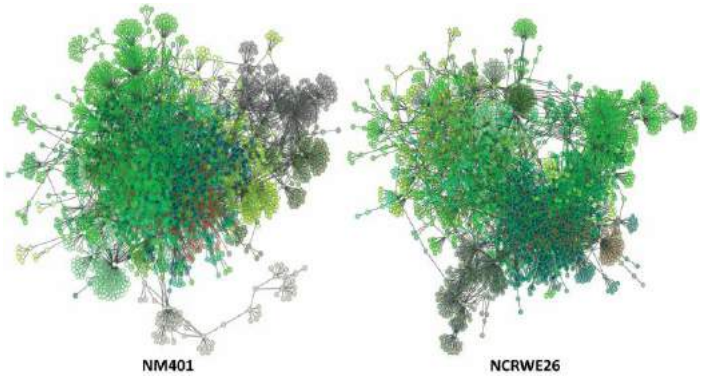
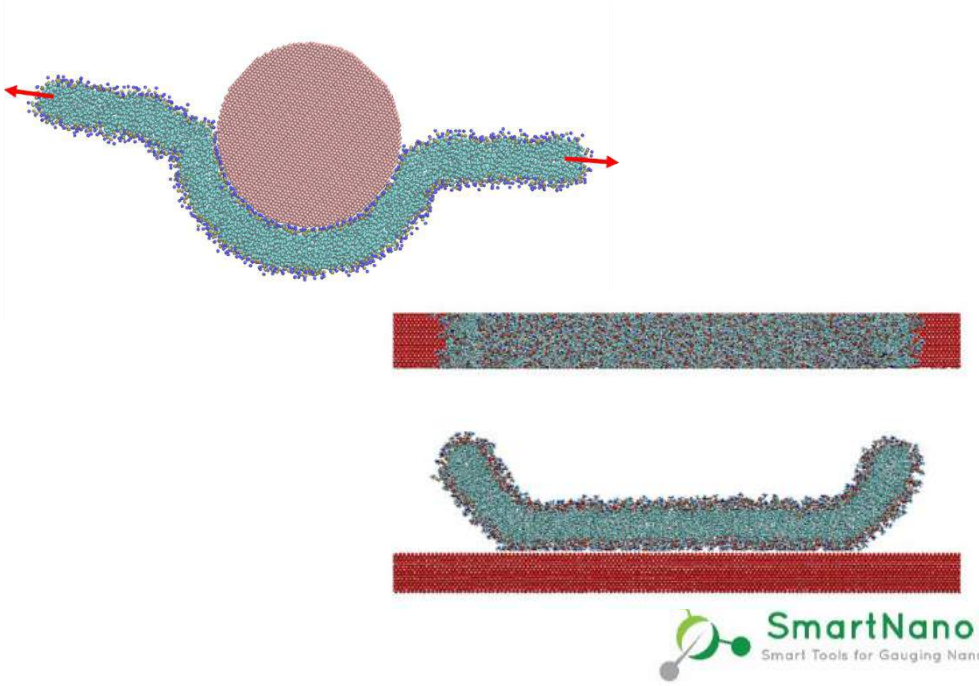
SmartNanoTox Data: in silico

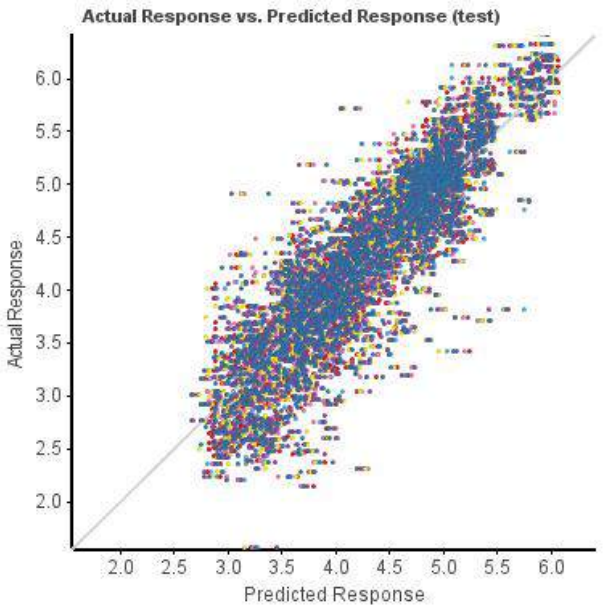


Binding free energies of aminoacids to NP

Outer corona surface defines further fate of NP







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SmartNanoTox Data: in silico

Study	Activity	Activity Description	Type of data for sharing	Shared Format	Archive
Proteins	Molecular simulation	Prediction of 3D structure of proteins using i-Tasser software, calculation of molecule characteristics	coarse-grained models, sequence descriptors, structure descriptors, adsorption energies	CSV*	SNT, Zenodo
NMs	Molecular simulation	Quantum-chemical modelling of NM, calculation of material properties	NM coarse-grained presentation, NM descriptors, Hamaker constants	CSV*	NanoCommons, Zenodo
AOP	Statistical Modelling	Computer simulation (CG) of the interaction of the key molecule with the NM	Programs & Computational models	Mathematica NB, ISA-TAB, JSON	SNT, Zenodo
NMs	Molecular simulations	Multiscale modelling of NM corona formation & validation of the modelling against in vivo studies	Bionano interactions descriptors - adsorption free energies; binding coordination	data sheets CSV*	SNT, Zenodo

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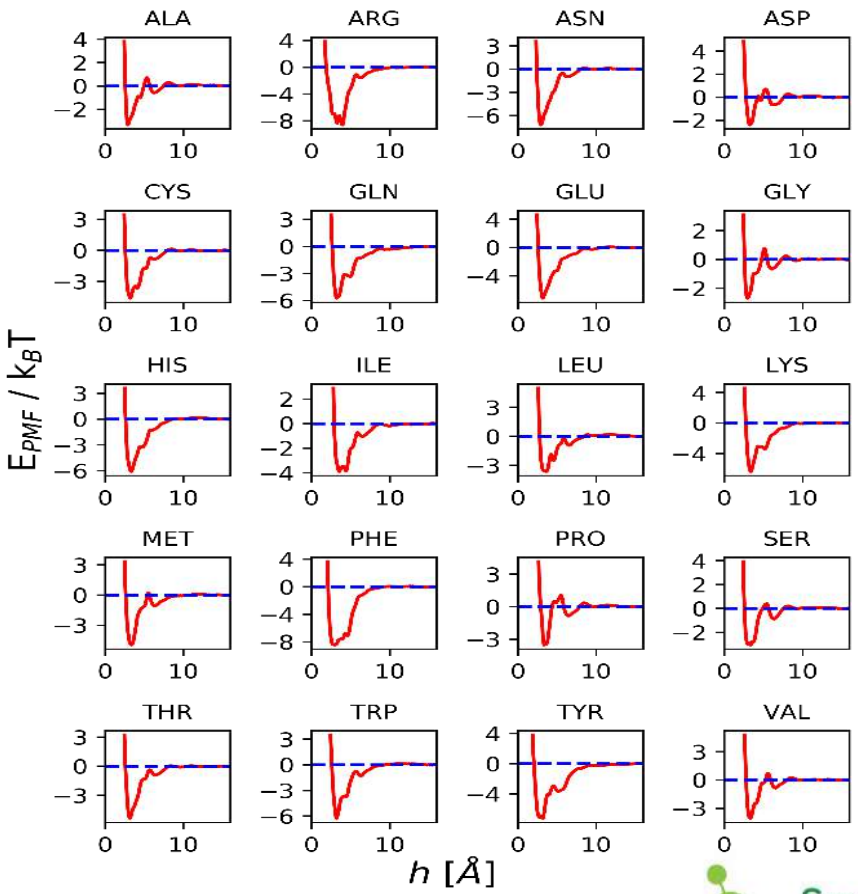
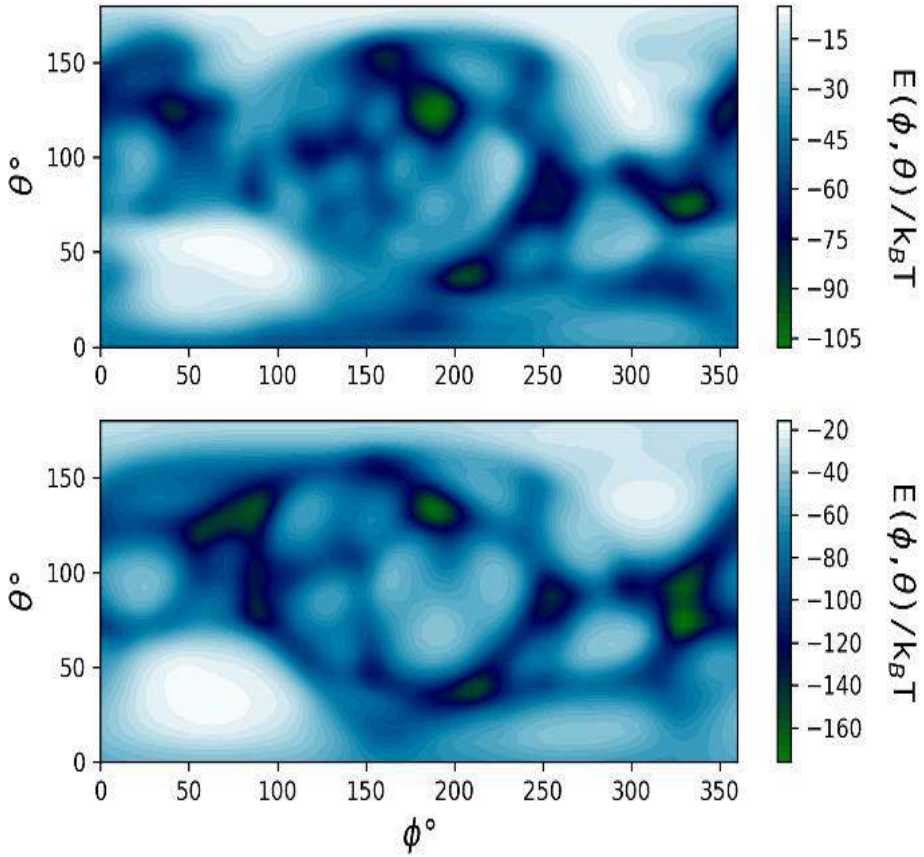
NM-protein interaction

Each material is linked to a set of 30 PMFs: amino acids, lipid fragments, sugars. Protein adsorption maps





NM-biomolecule interaction

Biomolecular segment / Protein adsorption (over 800 proteins) energies calculated

	A	B	C	D	E	AT	AU	AV	AW	AX	AY	AZ	BA	BB	BC	BD	BE
1			***Predictors***														
2	***Material***	***Allotrope***	***Miller Index***	***Size***	***Zeta***	***1b1i***	***1c1z***	***1ezq***	***1gpz***	***1htn***	***1ioj***	***1jmj***	***1kw2***	***1lfg***	***1lil***	***1mim***	***1n5u***
3	Au	FCC	100	2.5	-20	-147.0907799	-72.1658991	-158.7332988	-75.57572679	-110.3939673	-69.1695477	-164.1173805	-87.76523434	-116.545405	-100.0581262	-79.25384464	-91.31119205
4	Au	FCC	100	2.5	0	-135.6199959	-74.44987467	-163.8811221	-70.89634133	-108.2114499	-68.69490177	-155.0745482	-89.68902249	-110.0201813	-100.9717773	-80.51525054	-90.93538727
5	Au	FCC	100	2.5	20	-137.8753526	-73.15022555	-165.9051136	-74.49809888	-106.6061161	-68.30082129	-152.2855027	-92.25047033	-111.8365457	-101.7556203	-78.91844731	-90.24604588
6	Au	FCC	100	5	-20	-168.2344298	-122.8699972	-201.1748371	-133.2718288	-140.5250218	-107.6316017	-216.2817715	-154.1101643	-209.4624623	-128.3240055	-110.5771393	-136.4120741
7	Au	FCC	100	5	0	-154.5286275	-115.7026871	-199.0667568	-132.996349	-140.7023195	-108.5358072	-210.4788615	-156.0235425	-209.8981399	-122.9621732	-105.3491486	-138.5030444
8	Au	FCC	100	5	20	-153.6726683	-118.2132588	-207.00702	-127.800576	-144.9111324	-107.7846037	-212.9642228	-152.6916729	-203.5115334	-128.0268692	-107.7007551	-139.7954308
9	Au	FCC	100	10	-20	-170.9903584	-154.6101941	-213.8327004	-192.7501249	-166.0380276	-138.8264757	-277.6299845	-197.4210307	-264.6806944	-160.9334025	-184.56659	-194.8158176
10	Au	FCC	100	10	0	-168.8498117	-154.3107459	-199.0532365	-193.3650748	-163.5390214	-133.8138716	-280.67787	-195.6290917	-258.5199794	-161.6405926	-167.0512764	-193.3228309
11	Au	FCC	100	10	20	-166.904462	-150.5573289	-213.1533821	-190.8525571	-165.9941486	-135.1415004	-280.5036499	-194.6417379	-249.6514058	-157.780587	-155.7894826	-208.3308027
12	Au	FCC	100	20	-20	-182.3602361	-203.7680621	-227.69578	-215.2032931	-176.513006	-158.2806743	-294.0924062	-210.4951124	-284.9472049	-182.552345	-167.4110729	-243.7573254
13	Au	FCC	100	20	0	-178.3796116	-206.2206065	-225.7159402	-213.6743483	-172.1212883	-157.2197608	-303.30623	-221.4216527	-285.3727268	-181.2304994	-163.7429521	-231.950671
14	Au	FCC	100	20	20	-176.863928	-193.5464128	-228.5475	-211.5169702	-178.5486913	-156.8402722	-299.8766598	-214.0902758	-284.61372	-181.3233681	-163.121895	-239.8089045
15	Au	FCC	100	40	-20	-187.707032	-216.8949182	-231.4021306	-234.0306894	-181.3096916	-147.511269	-299.6602747	-220.9961386	-313.5209106	-197.2708501	-178.33786	-233.8563332
16	Au	FCC	100	40	0	-186.442287	-223.7261593	-227.5521762	-236.2955468	-181.5556702	-154.0755527	-310.98979	-224.3626554	-308.9565276	-196.5289989	-176.7610256	-231.5191033
17	Au	FCC	100	40	20	-190.1424025	-214.0921957	-228.9360157	-235.3124375	-192.2970927	-149.0602196	-298.7250055	-227.0651927	-300.0941777	-185.7608525	-179.73154	-234.3778068
18	Au	FCC	100	50	-20	-192.0761834	-233.0817855	-237.8384539	-247.9985343	-192.1529758	-153.7496805	-317.2810734	-229.0025838	-313.7211879	-196.7804151	-182.9305499	-239.3181627
19	Au	FCC	100	50	0	-191.1720749	-229.9924989	-232.1249372	-245.6063485	-196.4331648	-156.7704692	-300.6773714	-224.9017214	-318.01677	-195.9640086	-183.3321	-237.3638418
20	Au	FCC	100	50	20	-185.6093695	-235.7213823	-229.8664841	-243.997407	-189.1864977	-151.4625133	-296.2510058	-228.6035153	-310.1765583	-203.3407471	-177.0022095	-238.2711187
21	Au	FCC	100	80	-20	-200.3455005	-276.52093	-230.1166846	-254.9355481	-185.2199334	-160.6970747	-309.7321818	-228.3466152	-322.28586	-206.041843	-174.5519448	-233.0257675
22	Au	FCC	100	80	0	-195.6793906	-288.4753398	-233.519357	-255.5721914	-194.0422515	-154.040292	-300.6656366	-246.190259	-322.43613	-202.7543817	-178.0262751	-230.5736174
23	Au	FCC	100	80	20	-181.7882362	-267.6087434	-232.064804	-252.2727682	-191.8671357	-154.1218134	-300.9452536	-231.3464574	-317.18648	-201.9482488	-178.9348109	-250.6357611
24	Au	FCC	100	100	-20	-192.4114808	-259.3475114	-234.5641377	-252.4673758	-191.9987785	-154.4760746	-319.2716292	-233.5079656	-323.16092	-206.89238	-181.4334796	-214.5505851
25	Au	FCC	100	100	0	-189.0758158	-273.2205365	-229.8686812	-259.1395046	-190.2937038	-155.1879734	-305.7308948	-238.9588324	-301.8340298	-200.6001628	-172.3037136	-238.39551
26	Au	FCC	100	100	20	-188.7509439	-270.185731	-238.4078608	-252.7039523	-188.3982138	-154.2549162	-295.580856	-245.1605892	-306.603548	-201.6821998	-174.8435887	-244.8630197
27	CdSe	Wurtzite	2-10	2.5	-20	-0.397326013	-0.14213185	-0.269429693	-0.270205075	-0.15056452	-0.129092563	-0.563650328	-0.184735869	-0.406590988	-0.284908553	-0.307688592	-0.193155617
28	CdSe	Wurtzite	2-10	2.5	0	-0.192519687	-0.110983271	-0.219290946	-0.254393781	-0.184760905	-0.114798459	-0.389831653	-0.253930763	-0.350855444	-0.282879064	-0.25283901	-0.277500944
29	CdSe	Wurtzite	2-10	2.5	20	-0.042277791	-0.084342099	-0.209915668	-0.265369382	-0.239484143	-0.106523635	-0.321925541	-0.353391928	-0.362194838	-0.289639964	-0.209603768	-0.385746558
30	CdSe	Wurtzite	2-10	5	-20	-0.703400937	-0.396455042	-0.558896349	-0.687158732	-0.36150896	-0.241317781	-1.329008582	-0.492760055	-1.093753479	-0.606696125	-0.796405628	-0.522355606
31	CdSe	Wurtzite	2-10	5	0	-0.377518503	-0.320643745	-0.470029646	-0.627806492	-0.403866652	-0.211064107	-0.934077016	-0.627924022	-0.992641405	-0.602060956	-0.650679082	-0.712402321
32	CdSe	Wurtzite	2-10	5	20	-0.147281278	-0.257837272	-0.460648081	-0.683265791	-0.487599763	-0.192754428	-0.818746898	-0.845814826	-1.086035117	-0.61633953	-0.542994833	-0.973300891
33	CdSe	Wurtzite	2-10	10	-20	-0.968536766	-0.869554954	-0.838990418	-1.148162153	-0.677990797	-0.303742039	-2.149608531	-0.785597924	-2.028588993	-0.934227446	-1.334844712	-0.887189343
34	CdSe	Wurtzite	2-10	10	0	-0.541369314	-0.728065543	-0.713308312	-1.048752505	-0.680561823	-0.265397229	-1.526126523	-1.003575521	-1.95105307	-0.923557817	-1.074426138	-1.206546812
35	CdSe	Wurtzite	2-10	10	20	-0.245845027	-0.61143785	-0.702579806	-1.172251929	-0.756678779	-0.242246337	-1.379689782	-1.378397514	-2.310769551	-0.940238205	-0.874182739	-1.668906462
36	CdSe	Wurtzite	2-10	20	-20	-1.14589845	-1.623267951	-1.03693977	-1.59985867	-0.857355984	-0.327522958	-2.751901407	-0.96005075	-2.643904523	-1.160154991	-1.55888792	-1.124289804
37	CdSe	Wurtzite	2-10	20	0	-0.653660502	-1.392745507	-0.885214532	-1.499468203	-0.843842676	-0.288698259	-1.944680193	-1.245949294	-2.555511929	-1.135480965	-1.278728806	-1.561121615
38	CdSe	Wurtzite	2-10	20	20	-0.313912134	-1.220006102	-0.873381782	-1.695244602	-0.918691083	-0.264917701	-1.787964326	-1.7235934	-3.005354251	-1.14376579	-1.045142902	-2.158103362

NM Hydration and NM-lipid interaction

Atomistic MD simulations

	surface	Au 100	SiO_2 Q^2	SiO_2 Q^3	SiO_2 Q^{3a}	SiO_2 Q^4	TiO_2 anatase 101	TiO_2 anatase 100	TiO_2 anatase 001	TiO_2 rutile 110	TiO_2 rutile 100	TiO_2 rutile 001
H20	water hydrogen bond density (nm^{-2})	n/a	5.7 ± 0.3	8.3 ± 0.3	6.5 ± 0.3	1.2 ± 023	6.3 ± 0.2	8.8 ± 0.3	5.1 ± 0.3	5.9 ± 0.1	10.9 ± 0.5	9.1 ± 0.5
	immersion enthalpy ($mN.m^{-1}$)	n/a	-76.7 ± 0.8	-151 ± 1.5	-117± 2	22.2 ± 0.8	-774 ± 1	-1176 ± 1	-542 ± 1	-1024 ± 1	-1009 ± 1	-1149 ± 1
	adsorption energy ($kJ.mol^{-1}$)	-262.9	-2.5	-15.8	-3.8	-53.6	-2.3	-3.3	n/a	-2.2	-2.4	n/a
	adsorption enthalpy ($kJ.mol^{-1}$)	n/a	9.1 ± 8.3	-21 ± 6.9	-69 ± 11	-64.8 ± 9.1	n/a	n/a	n/a	n/a	n/a	n/a
lipid	area per lipid (nm^{-2})	0.84	0.65	0.67	0.71	0.64	0.65	0.65	0.62	n/a	n/a	n/a
	separation (nm)	0.36	0.76	0.54	0.52	1.01	0.87	0.84	1.15	n/a	n/a	n/a
	thickness (nm)	2.83	3.15	3.08	2.98	3.18	3.04	3.07	3.20	n/a	n/a	n/a
	adhesion strength ($mN.m^{-1}$)	-42.2 ± 2	-0.8 ± 0.3	-1.2 ± 0.3	-2.7 ± 0.5	-0.7 ± 0.2	-3.3 ± 0.3	-6.6 ± 0.7	0	>0	>0	>0
	adhesion enthalpy ($mN.m^{-1}$)	-118 ± 7.4	2.1 ± 1.2	-2.8 ± 1.7	-10 ± 1.1	-3.4 ± 2.1	-5.5 ± 1.3	n/a	n/a	n/a	n/a	n/a

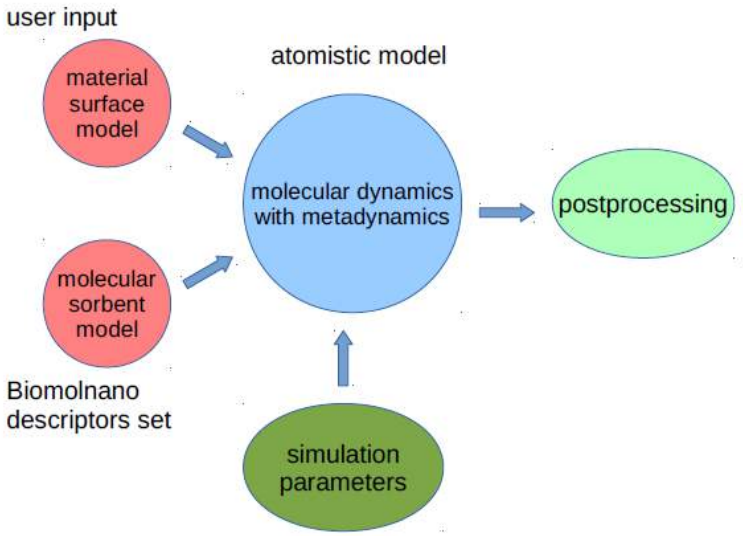
MODA Workflow: bionano interaction PMF

in certain class of solvers for the models.

Sim

3	Specific Computational Modelling Metadata		
3.1	Numerical Solver	Verlet algorithm with V-rescale thermostat Well-tempered metadynamics algorithm with collective variable determined as the surface separation distance between the sorbent molecule and surface	
3.2	Software Tool	Gromacs v. 5.1.2 with Plumed 2.3	
3.3	Time Step	2 fs, total simulation time ~300 ns	
3.4	Computational Representation *Refers to how your computational solver represents the material, properties, equation variables,*	Physics Equation, Material Relations, Material	Newton's equations are discretized in a Verlet scheme. Forces are computed by summation over all atom pairs within the cut-off radius. Long-range electrostatic interactions are treated by the Particle Mesh Ewald (PME) Well-tempered met
3.5	Computational Boundary Conditions	Material slab periodic in X and Y di Water filling the rest of the simulat	
3.6	Additional Solver Parameters	thermostat relaxation time: 1 ps real space cutoff: 1 nm PME grip spacing: 0.1 nm preequilibration time: 1 ns initial height of Gaussians: 2.5 kJ/n bias factor: 15 Additional potential wall for the so $U_{wall}(s)=k(s-a)^4$ with the force constant k = 40 kJ/(n	
3.7	Publications	E. G. Brandt and A. P. Lyubartsev "N Amino Acid Side Chain Analogues a Surface" J. Phys. Chem. C, 119(32),	

Workflow picture



SmartNanoTox
Smart Tools for Gauging Nano Hazards

Challenges

- Absence of ontologies for novel in vitro, in silico methods and outcomes
- Non-conventional methods and data types

Semantic mapping
simulation ↔ experiment

- Level 1: bulk material (chemistry + crystalline form) → NM
- Level 2: nanomaterial model (L1 + specific size + basic extrinsic properties (charge) → NM
- Level 3: nanomaterial model (L2 + size distribution + extrinsic properties (coating)) → NM

Further actions

July-September 2020

- Data organisation and storage – SNT server, GEO, Zenodo
- In vivo/ in vitro data conversion and annotation: TA NanoCommons
- In silico data: data organisation and storage, semantic mapping – NanoCommons

2020-2021

- Models: integration into NanoCommons KB, NanoSolveIT KB, Biovia QSAR WorkBench, Biovia Materials Studio
- All data release to public