eNanoMapper

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U.S.-EU: Bridging NanoEHS Research Efforts
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(on behalf of...)

These slides are mine and may not fully reflect the opinion of all partners.

Goal NMP-2013.1.3-2: Nanomaterial Safety Assessment

- Ontology …
  - what are we talking about
  - minimal reporting standards
- Database(s) …
  - all content described with ontologies
  - interoperate with and link to other databases
- … for modelling and risk assessment
  - API needed for database

- Community Embedding
  - solve real needs

Karolinska Institutet

VTT

Maastricht University Leading in Learning!

EMBL-EBI

Douglas Connect GmbH, Switzerland

in silico toxicology gmbh

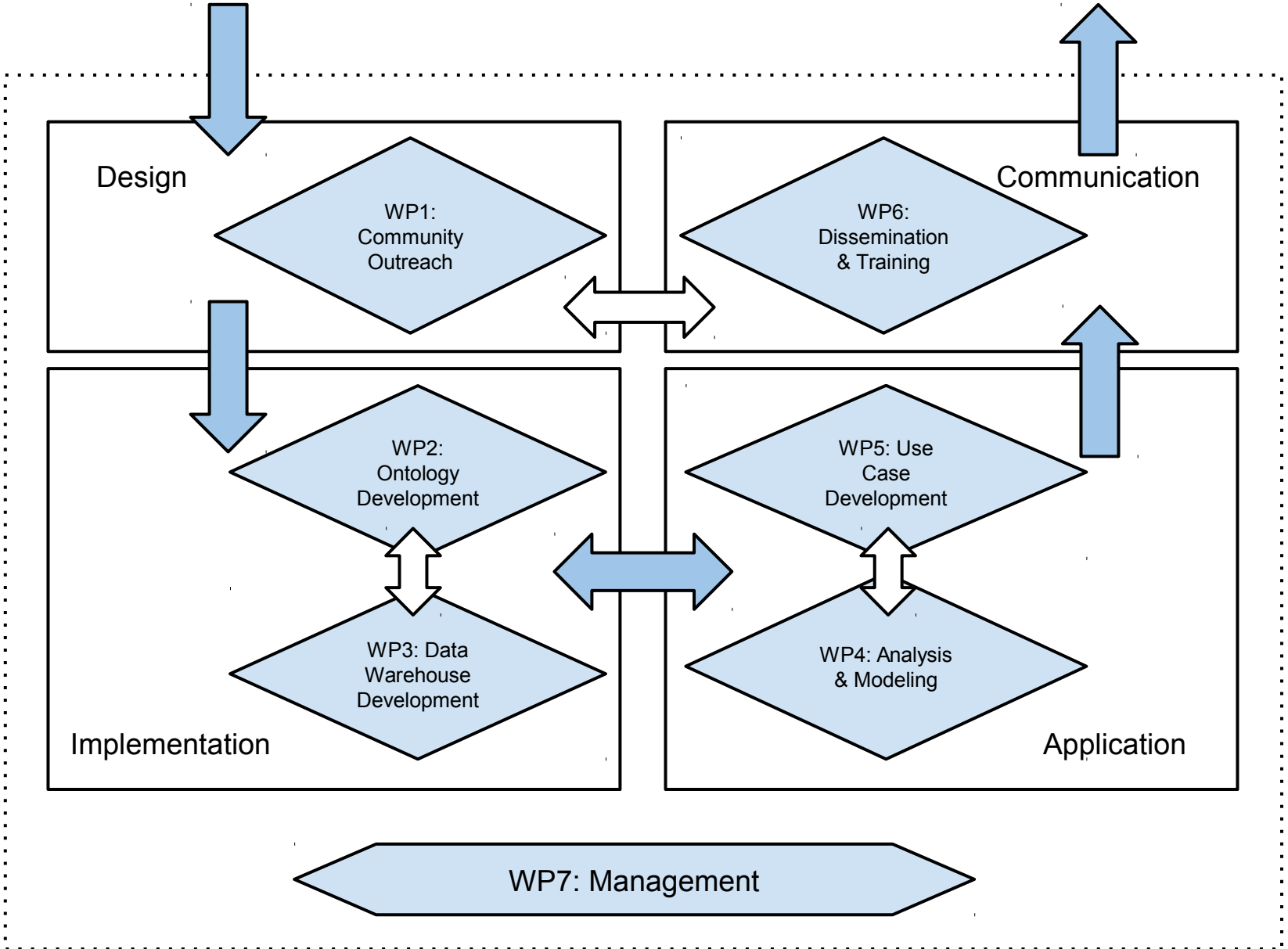
IOEA consult

Nat. Tech. Univ. of Athens, Greece

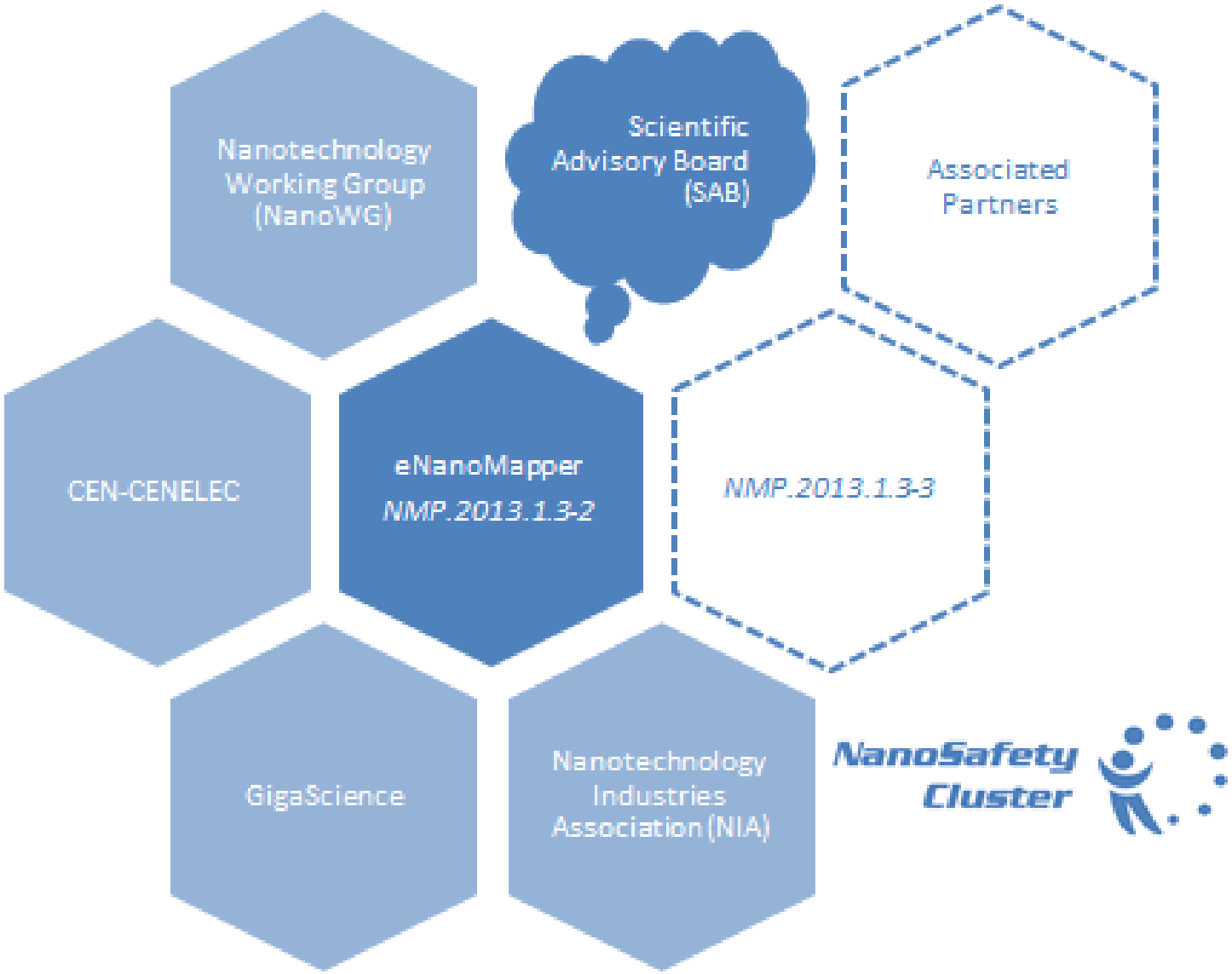
What we envision…

1. (re)use (open) ontologies
   - CHEMINF, NPO, BAO, QUDT, …
2. based on OpenTox
   - EU FP7 projects: OpenTox, ToxBank
   - Open Source implementations (incl. AMBIT)
3. Application Programming Interfaces (APIs)
   - allow bridging with data analysis tools
   - exchange formats: ISATab, RDF, ...

Work packages



Community Embedding



A sketch: Based on OpenTox ...

ambit

SMARTS

Keywords

Search

Search for substructure and properties

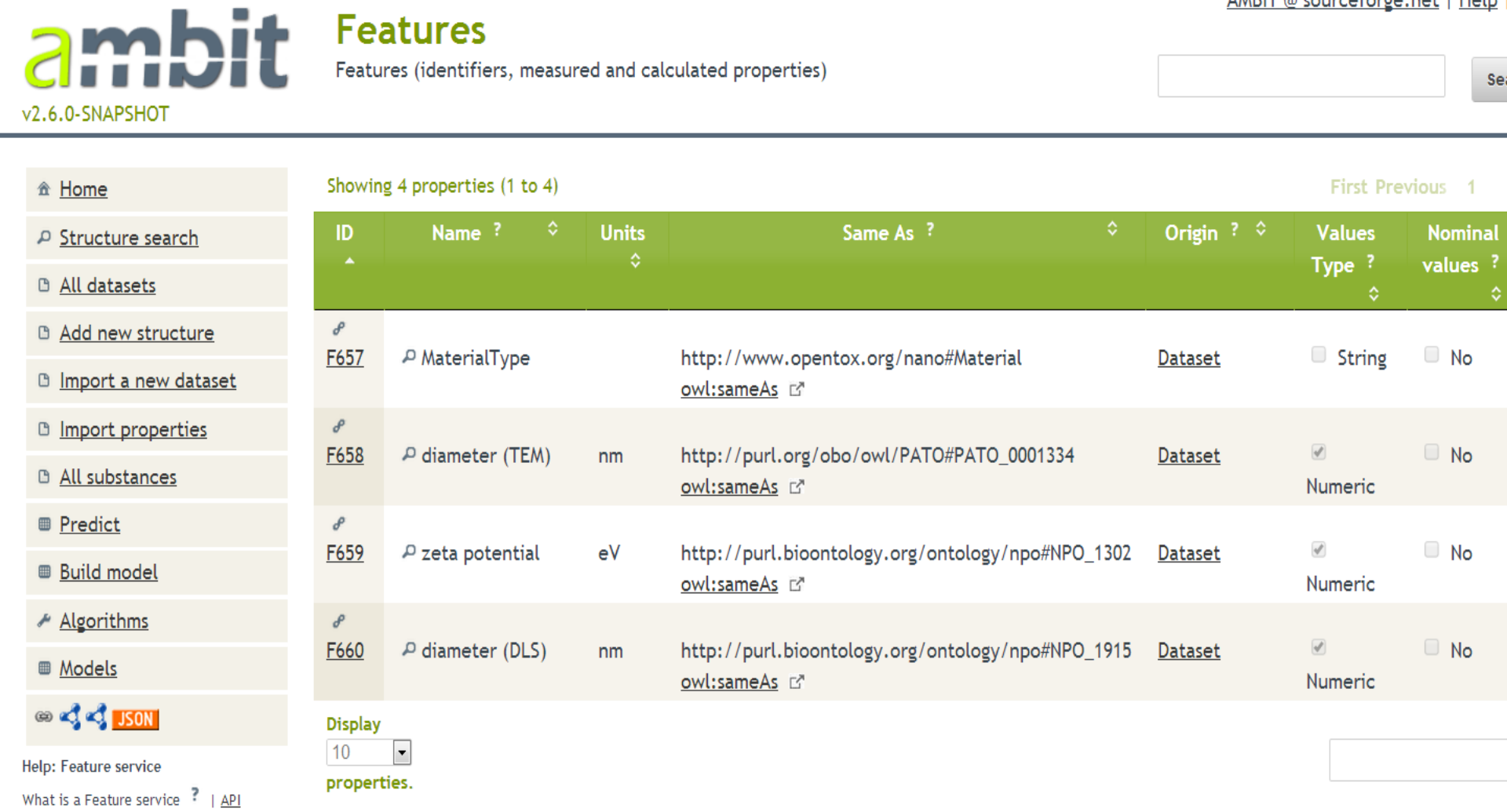
This dataset | License | Show: Structure diagrams | Identifiers | Names | SMILES | InChI | Endpoints | Calculated | Properties | Similarity |
Download as JSON |
Page 0 Page size 100

Showing 11 structures (1 to 10)

First Previous 1 2 Next Last

			MaterialType	diameter (TEM) nm	zeta potential eV	diameter (DLS) nm
	1.	NanoMaterial	METALOXIDE	14.7	-24	524.8
	2.	NanoMaterial	METALOXIDE	12.8	-28.9	321.3
	3.	NanoMaterial	METALOXIDE	18.3	-25.5	378.3
	4.	NanoMaterial	METALOXIDE	10	-29	247.6

Semantic Predictive Toxicity



bit

Substance study

Mono-constituent, multiconstituent, additives, impurities.

Enter substance I5 UUID

Search

Composition | P-Chem (2) | Env Fate (3) | Eco Tox (4) | Tox (2)

Filter...

TO_BIODEG_WATER_SCREEN_SECTION (3)

Name	Conditions	Effects		Interpretation	Protocol		
	Time Point	Endpoint	Result	Result	Guidance	Owner	UUID
Biodegradation in water: screening tests, IUC4#1/Ch.3.5	28 d	% Degradation	= 90%	-	OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	IUC4 TODO	IUC4-1d75f...
Biodegradation in water: screening tests.001	3 h	% Degradation	= 0%	readily biodegradable	OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	IUC4 TODO	IUC5-2ea8...
	7 d	% Degradation	= 20%				
	14 d	% Degradation	= 50%				
	28 d	% Degradation	= 85%				
Biodegradation in water: screening tests.002	3 h	% Degradation	= 9%	inherently biodegradable	N/A	IUC4 TODO	IUC5-69bc...
	7 d	% Degradation	= 40%				
	14 d	% Degradation	= 50%				
	28 d	% Degradation	= 80%				

Showing 1 to 3 of 3 entries

Previous Next

erial with a definite
CH guide
multi-constituent ?
ent ? Additive ?

Application Programming Interfaces

Bioclipse Scripting Language

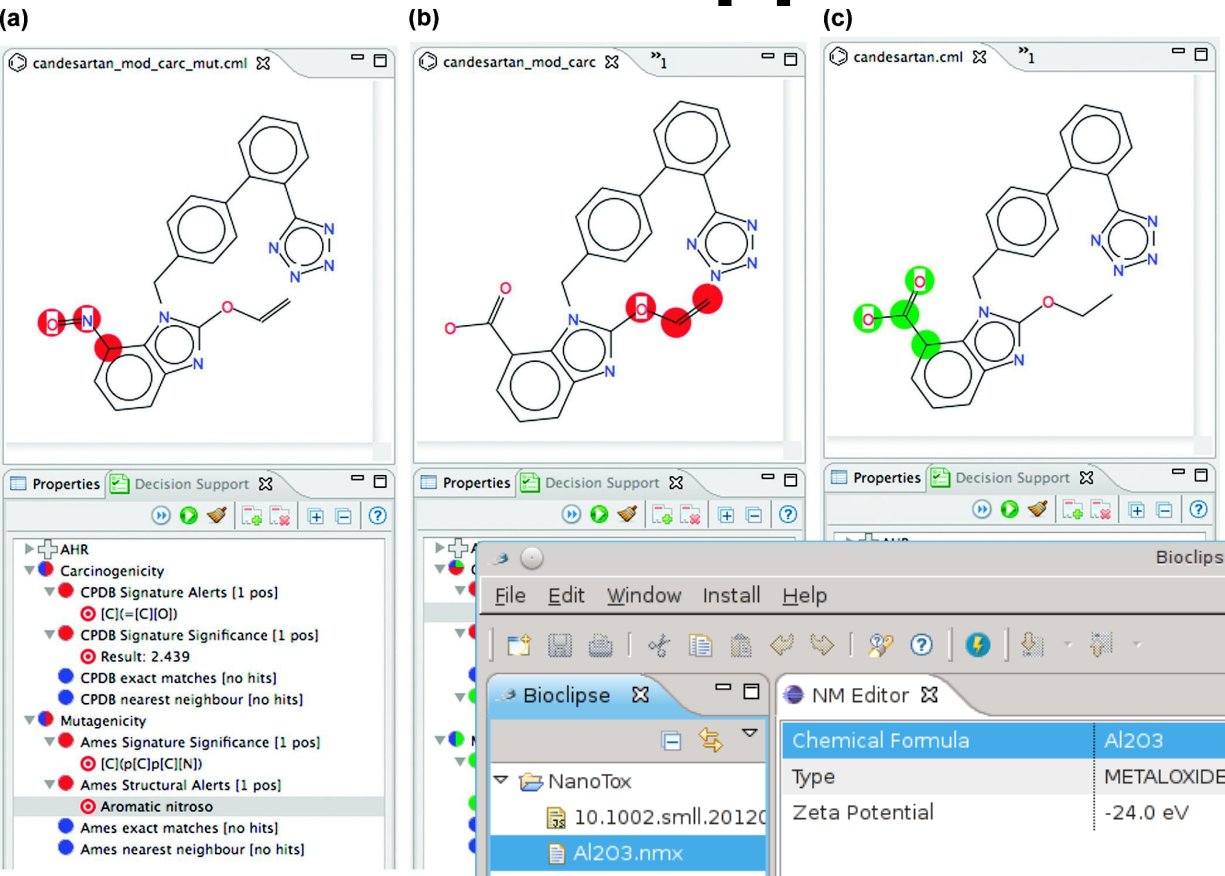
(JavaScript)

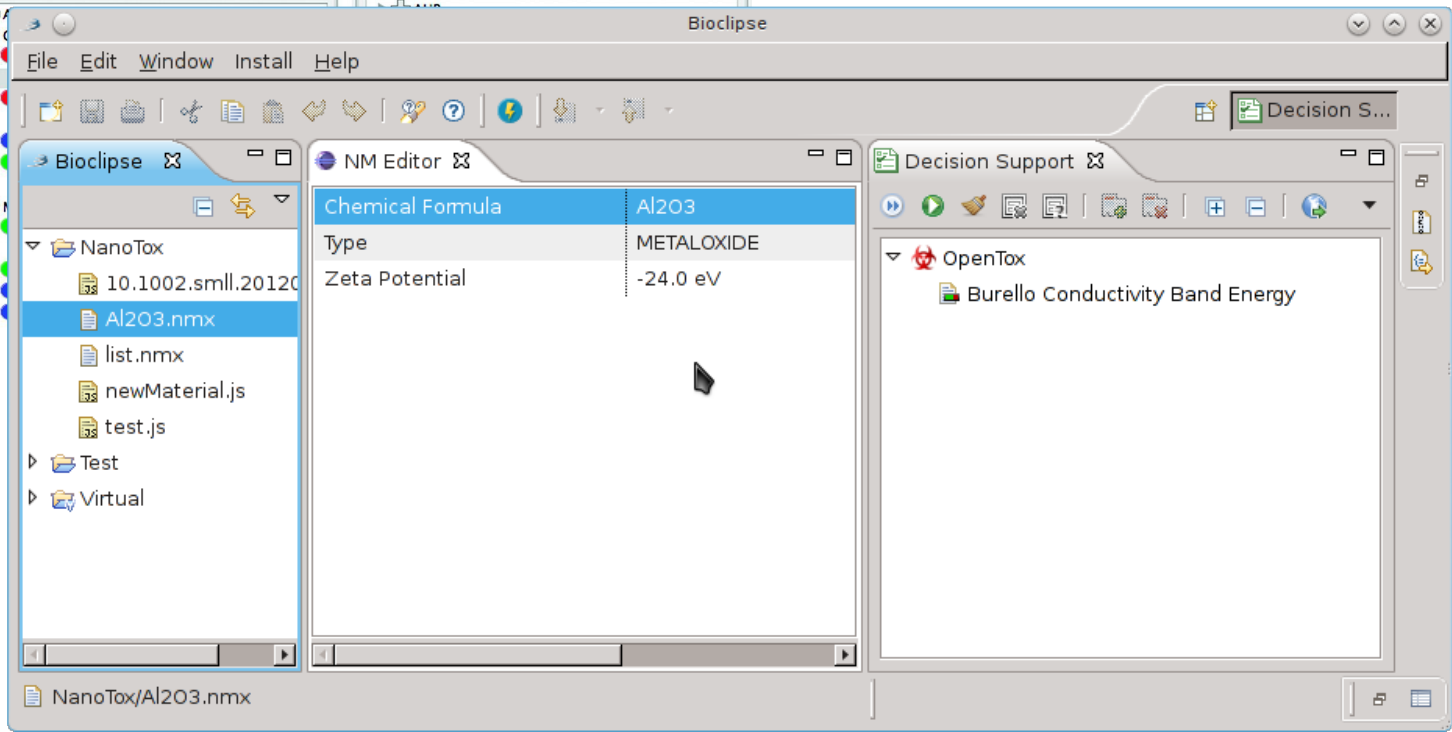
```
// data from: doi:10.1002/smll.201202128

materials = [
  [ "metal oxide", "Al2O3", 14.7, 5.2, "nm", 524.8, 32.8, "nm", -24.0, 0.5, "eV"],
  [ "metal oxide", "CeO2", 12.8, 3.4, "nm", 321.3, 8.6, "nm", -28.9, 3.3, "eV"],
  [ "metal oxide", "CoO", 18.3, 6.8, "nm", 378.3, 16.4, "nm", -25.5, 1.3, "eV"],
  [ "metal oxide", "Co3O4", 10.0, 2.4, "nm", 247.6, 16.9, "nm", -29.0, 2.2, "eV"],
  [ "metal oxide", "Cr2O3", 71.8, 16.2, "nm", 478.5, 7.2, "nm", -26.2, 3.1, "eV"],
  [ "metal oxide", "CuO", 193.0, 90.0, "nm", 289.5, 31.0, "nm", -26.9, 0.8, "eV"],
  [ "metal oxide", "Fe2O3", 12.3, 2.9, "nm", 385.2, 6.3, "nm", -24.1, 2.0, "eV"],
  [ "metal oxide", "Fe3O4", 12.0, 3.2, "nm", 831.7, 41.8, "nm", -27.0, 2.3, "eV"],
  [ "metal oxide", "Gd2O3", 43.8, 15.8, "nm", 726.7, 54.8, "nm", -34.7, 0.7, "eV"],
  [ "metal oxide", "HfO2", 28.4, 7.3, "nm", 349.9, 5.2, "nm", -24.3, 2.1, "eV"],
  [ "metal oxide", "In2O3", 59.6, 19.0, "nm", 303.2, 5.2, "nm", -35.5, 2.4, "eV"]
]
properties = [
  [ "diameter (TEM)", 2, 3, 4 ],
  [ "diameter (DLS)", 5, 6, 7 ],
  [ "zeta potential", 8, 9, 10 ],
]

list = nm.createList();
for (var i=0; i<materials.length; i++) {
  material = nm.newMaterial(materials[i][0]);
  nm.setComposition(material, materials[i][1]);
  for (var p=0; p<properties.length; p++) {
    nm.addCharacterizationValue(
      material, properties[p][0],
      materials[i][properties[p][1]], materials[i][properties[p][2]],
      nm.getUnitBySymbol(materials[i][properties[p][3]])
    )
  }
  nm.save(material, "/Virtual/" + materials[i][1] + ".nmx");
  list.add(material);
}
list;
opentoxnm.predictWithModel(
  "http://apps.ideaconsult.net:8080/bioclipse/",
  "http://apps.ideaconsult.net:8080/bioclipse/model/22",
  list
)
opentoxnm.calculateDescriptor(
```

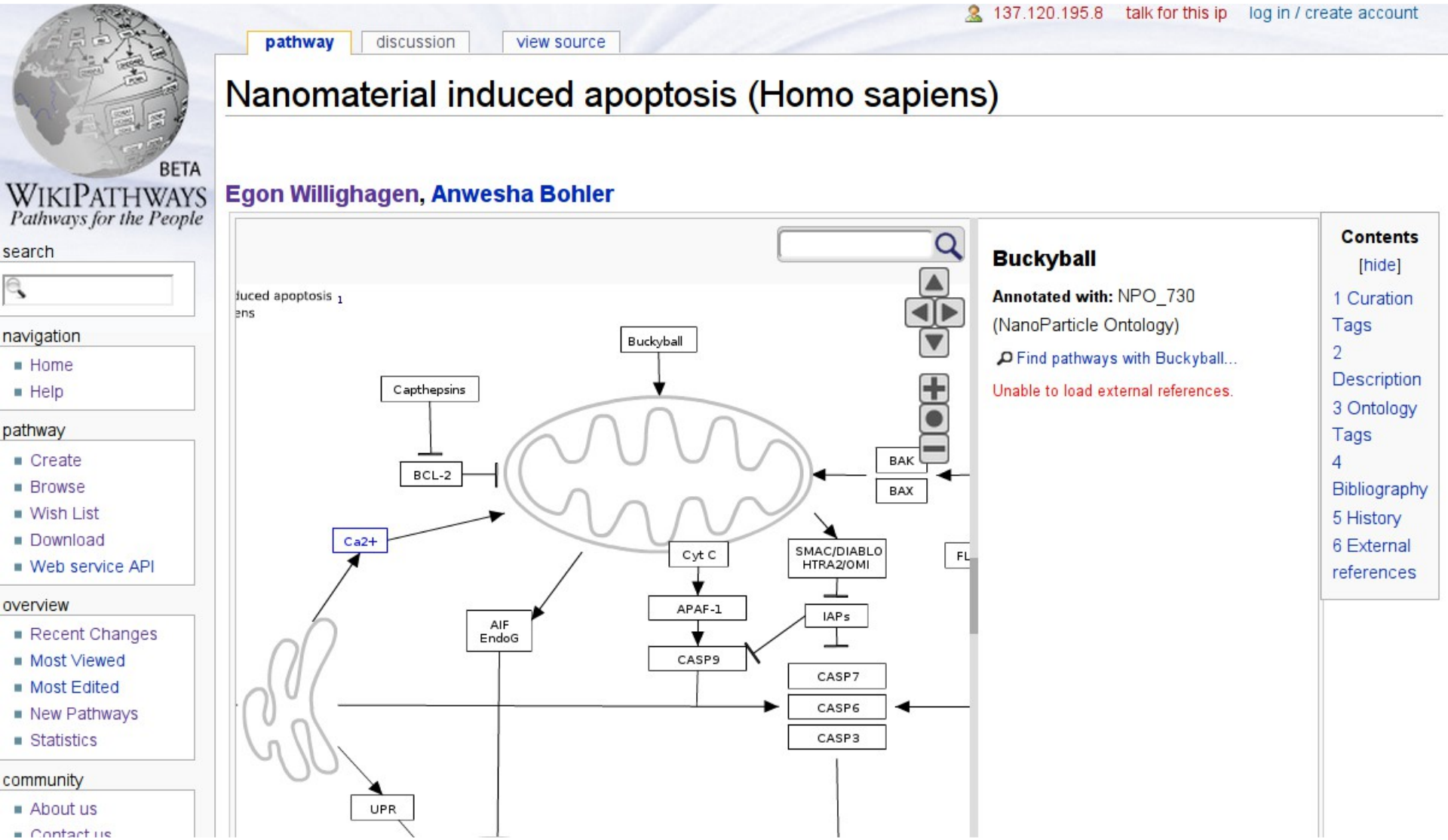
Decision Support





Ola Spjuth, et al.
JCIM, 2011, doi:
10.1021/ci200242c

Systems Biology: pathways



Andón FT, Fadeel B; "Programmed Cell Death: Molecular Mechanisms and Implications for Safety Assessment of Nanomaterials."; Acc Chem Res, 2012

Thanks

- eNanoMapper partners
  - see 4th slide
- AMBIT/OpenTox - NM - Bioclipse integration
  - dr Nina Jeliazkova (IdeaConsult Ltd.)
  - dr Ola Spjuth (Uppsala University, GenettaSoft)

Some reading material from my side:

1. E.L. Willighagen et al., Computational toxicology using the OpenTox application programming interface and Bioclipse, BMC Research Notes, 2011, doi:10.1186/1756-0500-4-487
2. O. Tcheremenskaia et al., OpenTox predictive toxicology framework: toxicological ontology and semantic media wiki-based OpenToxipedia, J. Biomed. Sem., 2012, doi:10.1186/2041-1480-3-S1-S7
3. C. Steinbeck et al., The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics. J. Chem. Inf. Comput. Sci, 2003, doi:10.1021/ci025584y
4. J. Hastings et al., The Chemical Information Ontology: Provenance and Disambiguation for Chemical Data on the Biological Semantic Web, PLOS ONE, 2011, doi:10.1371/journal.pone.0025513