Nanomaterial data visualization with ambit.js and d3.js
API Overview

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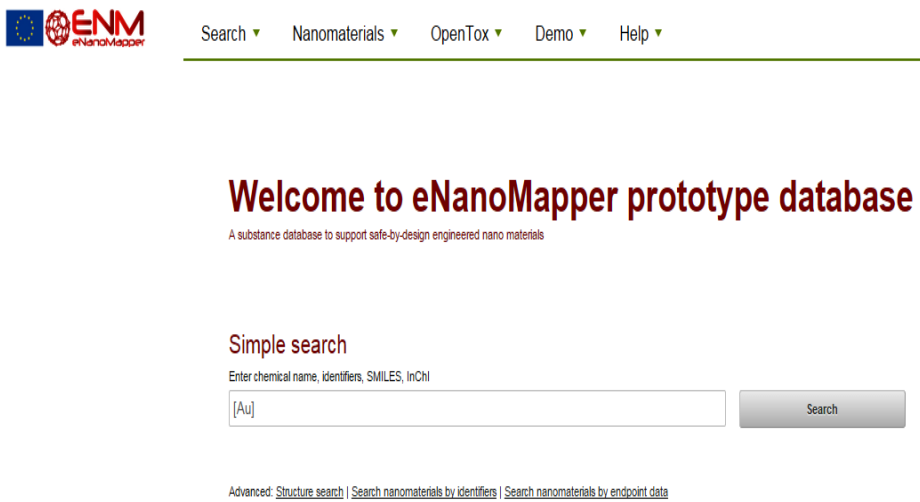
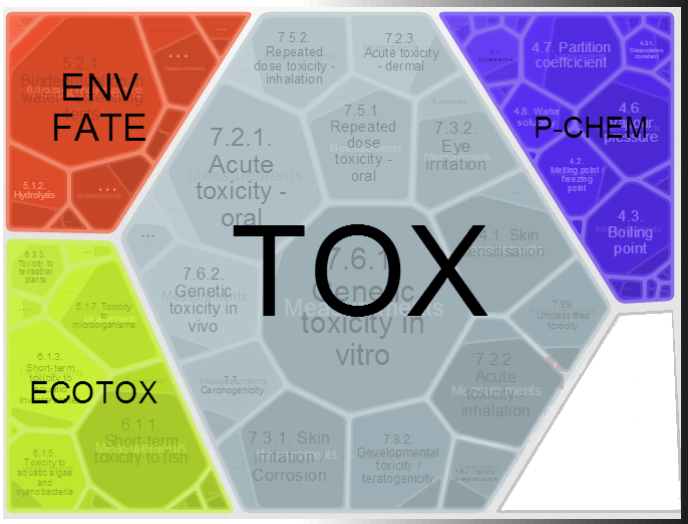
www.enanomapper.net

18 May 2015 webinar

eNanoMapper database
data.enanomapper.net

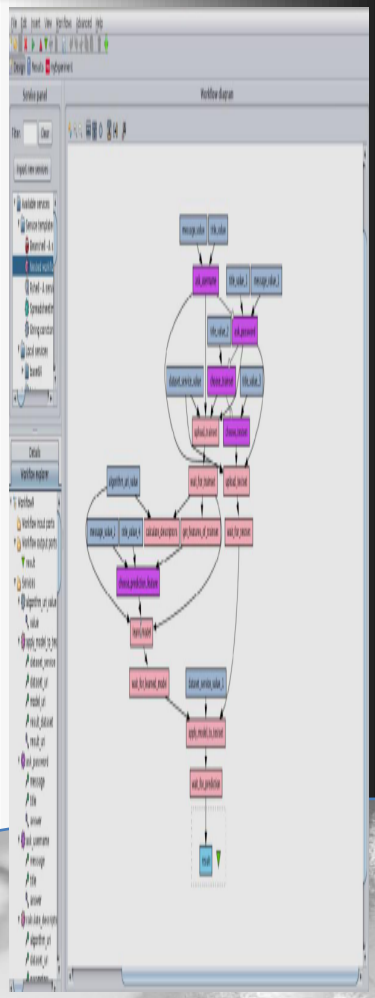




Jeliazkova, N., et al. The first eNanoMapper prototype: A substance database to support safe-by-design. In: Bioinformatics and Biomedicine (BIBM), 2014 IEEE International Conference on. IEEE, pp. 1-9. URL http://dx.doi.org/10.1109/bibm.2014.6999367

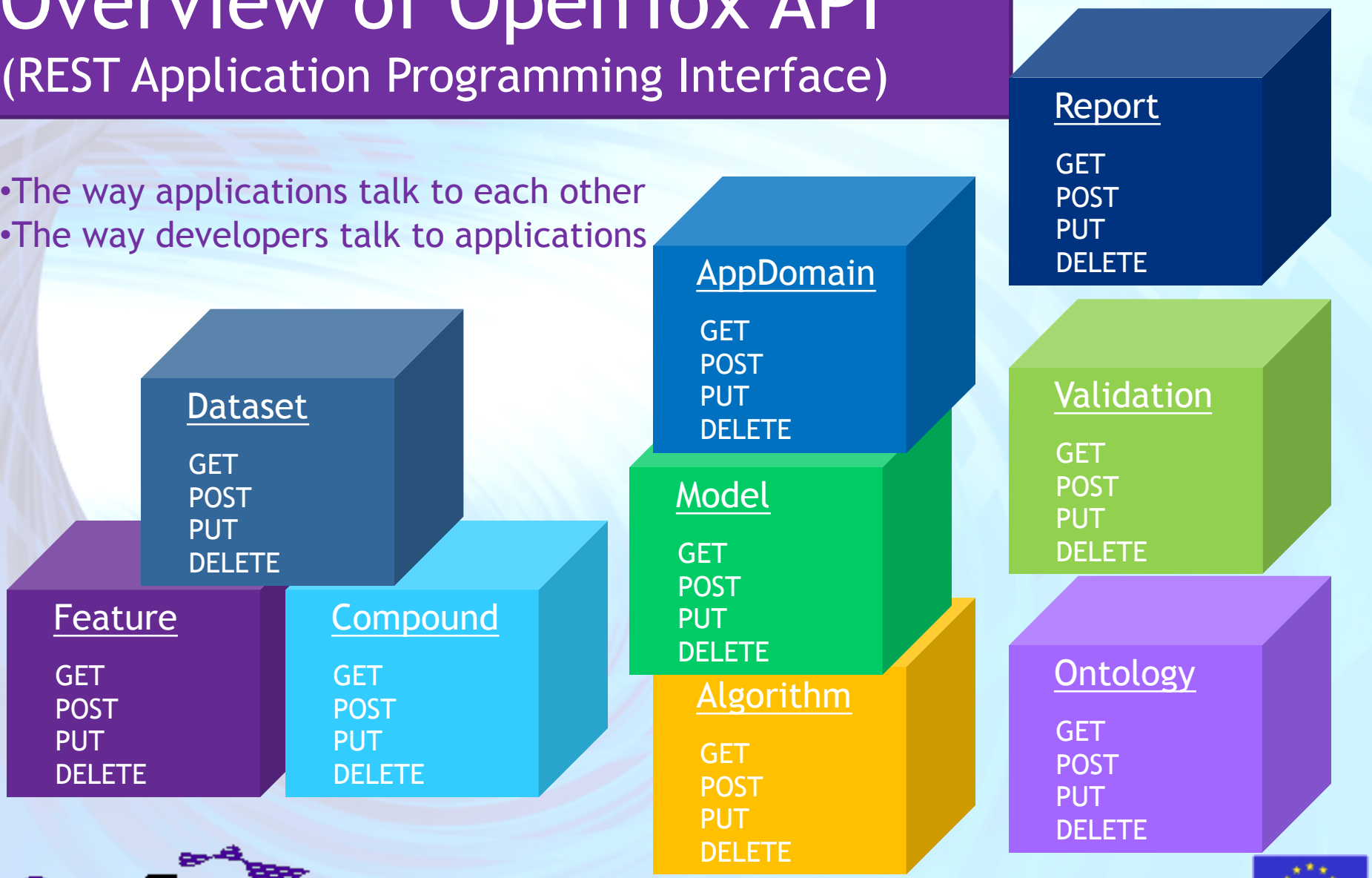
Application Programming Interface (API)

- API: A way computer programs talk to one another.
  - *Can be understood in terms of how a programmer sends instructions between programs*
- The API specifies how software components should interact
  - *A good API makes it easier to develop a program by providing all the building blocks. A programmer then puts the blocks together.*
- Access the database via
  - *Any programming language*
  - *Workflow systems : Taverna, Knime, Pipeline Pilot*
  - *Allow bridging with data analysis tools*
  - *Build different user interface and visualisations*
- Implement
  - *Your database with different technology but exposing the same API*
  - *Ideally multiple independent interoperable implementations*



Overview of OpenTox API
(REST Application Programming Interface)

- The way applications talk to each other
- The way developers talk to applications

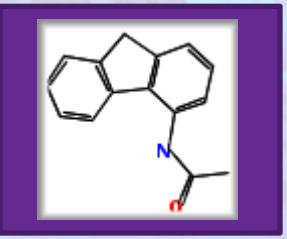


OpenTox

OpenTox datasets: Unified access to data

Everything described by W3C RDF (Resource Description framework)

Compound/ Data	http://myhost.com/feature/21580	http://myhost.com/feature/21589	http://myhost.com/feature/21573	http://myhost.com/feature/21576	http://myhost.com/feature/21588	http://myhost.com/feature/21858	http://myhost.com/feature/22114
http://myhost.com/compound/413	N,N-dimethyl-4-aminoazobenzene	CN(C1=CC=C(C=C1)N=N/C2=CC=CC=C2)C	3	3.31	225.3	YES	3.123
http://myhost.com/compound/44497	4-acetamidofluorene	O=C(Nc3					
...	...						



http://myhost.com/feature/21573

http://myhost.com/feature/21858

http://myhost.com/feature/22114

a ot:Feature , ot:NumericFeature ;
dc:creator
"http://www.blueobelisk.org/ontologies/chemoinformatics-algorithms/#xlogP" ;
dc:title "XLogP" ;
ot:hasSource
<http://myhost.com/algorithm/org.openscience.cdk.qsar.descriptors.molecular.XLogPDescriptor> ;
= otee:Octanol-water_partition_coefficient_Kow .

NM database challenges

- **Physico chemical identity**

Different analytic techniques, manufacturing conditions, batch effects, mixtures, impurities, size distribution, differences in the amount of surface modification, etc.

- **Biological identity**

Wide variety of measurements, toxicity pathways, effects of ENM coronas, modes-of-action, interactions (cell lines, assays).

- **Data formats, Provenance, Visualisation**

From raw data to study summaries for regulatory purposes; linking with experimental protocols; user friendly visualisation.

- **Diverse requirements, posed by the nanotechnology community;**
- **Data representation and integration challenges mainly due to data complexity and provenance**
- **Support for data analysis**

➢ Requires “spreadsheet” or matrix view of data.

➢ The experimental data in the public datasets is usually are not in a form appropriate for modelling.

➢ Standardisation in these sources is specific to each database.

➢ Even in curated collections the preparation of data for modelling is not a straightforward exercise

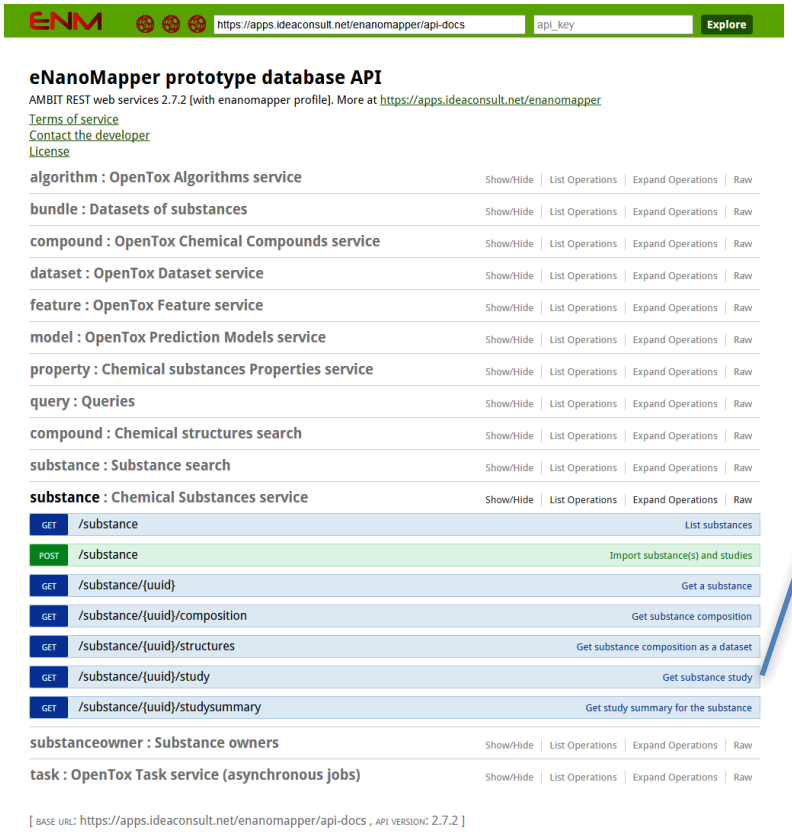
  ➢ (e.g. the experimental values can be merged in many different ways into a matrix, depending on which experimental protocols and conditions are considered similar; also there could be multiple values due to replicates or similar experiments)

Nanomaterials representation

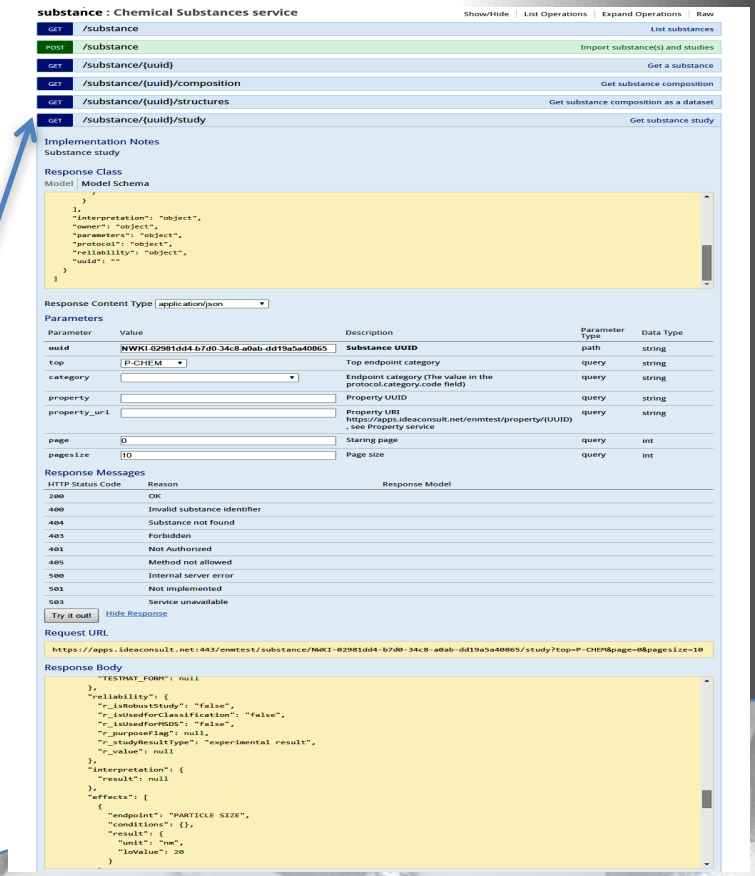
- Nanomaterials
  - Core
  - Coating(s)
  - Linkage
  - Impurities
  - Components, internal structure, etc.
- Typical assay description
  - Property – value (range of values) – units *(Excel templates)*
- More complex description:
  - Experimental graph *(ISA-TAB / ISA-TAB-nano)*
- Existing data models
  - *BioAssay Ontology*
  - *OECD Harmonized Templates*
  - *CoDATA UDS*
  - *ISA-TAB- Nano*
- Commonalities:
  - Materials sample
  - Protocols, protocol parameters
  - Experimental conditions
  - Readouts
    - Measurements,
    - Measurement groups,
    - Raw data, derived data

REST Application Programming Interface http://enanomapper.github.io/API/

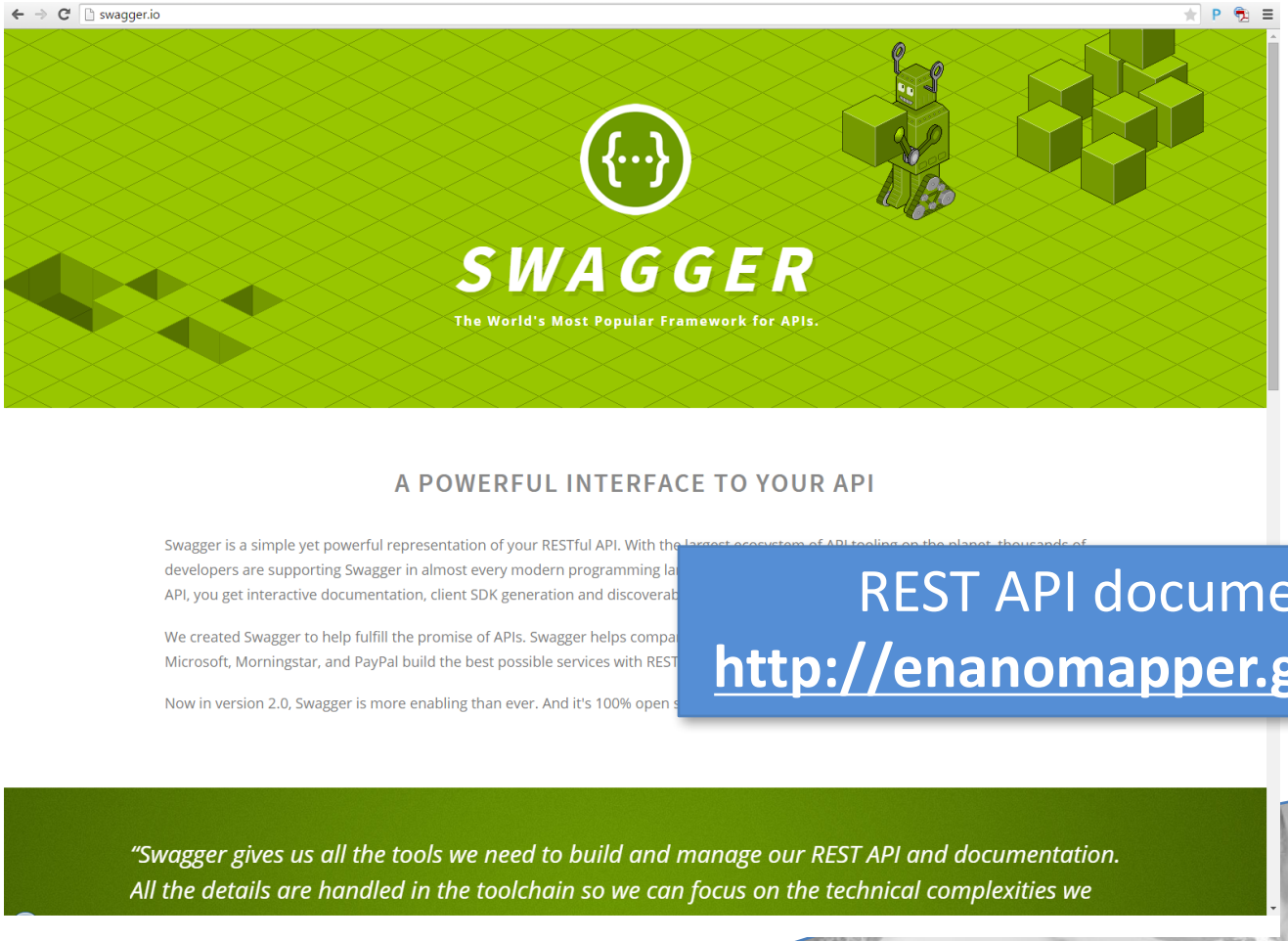
API documentation (Swagger-UI)



Interactive API queries



API documentation with Swagger

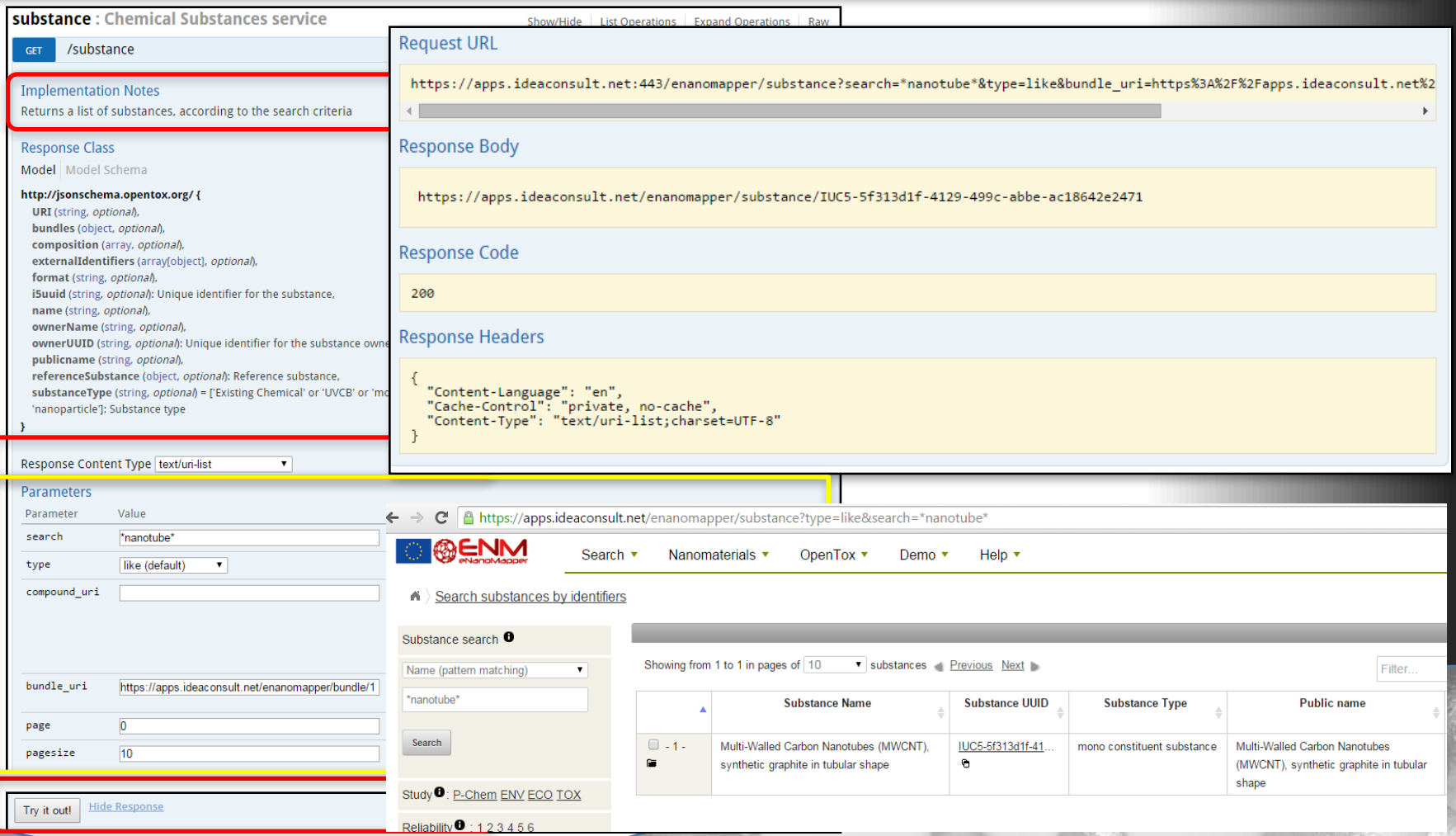


REST API documentation:
http://enanomapper.github.io/API/

eNanoMapper

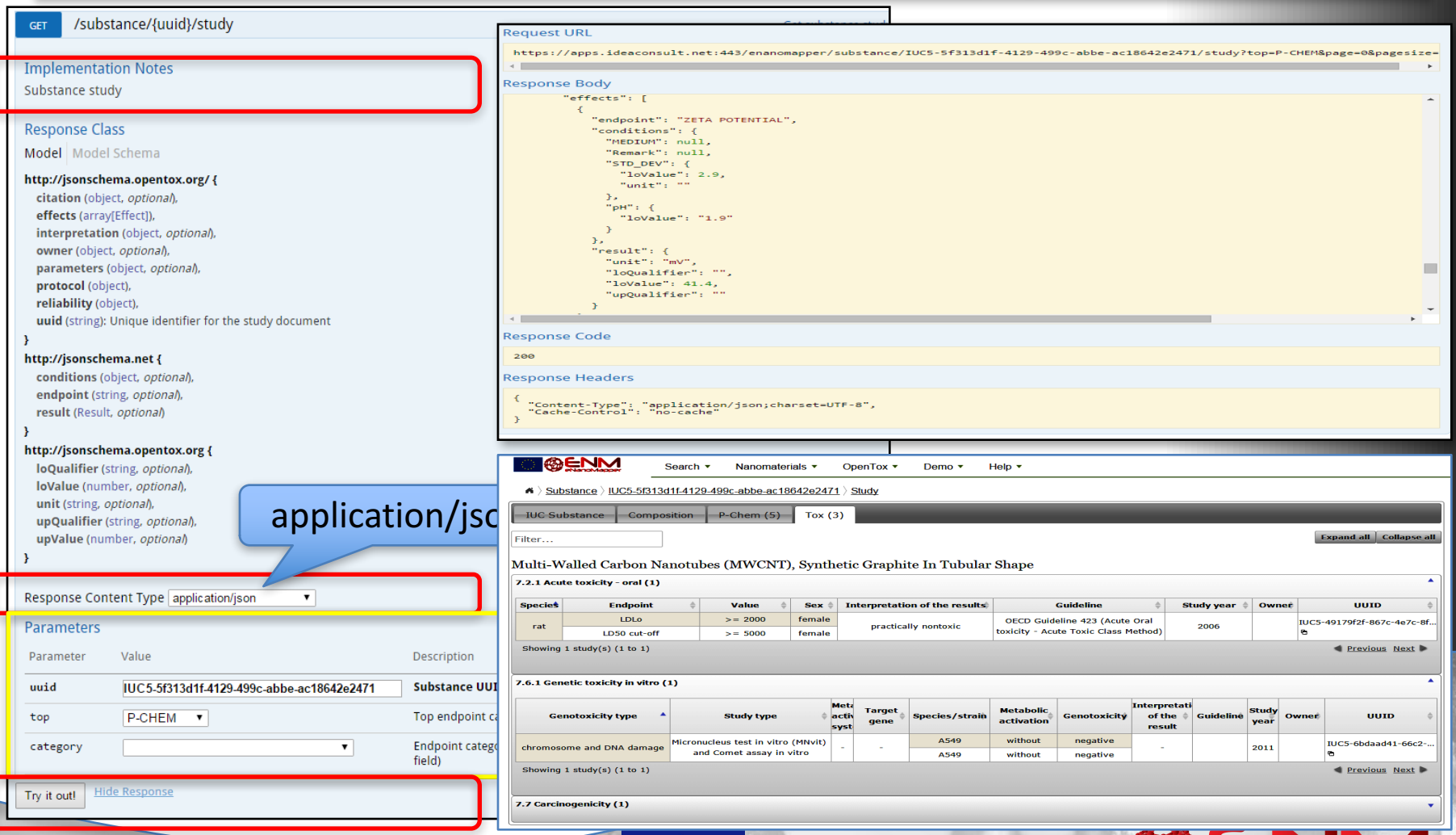
Substance search

http://enanomapper.github.io/API/#!/substance_1/getSubstances



Experimental data

http://enanomapper.github.io/API/#!/substance_1/getSubstanceStudy



Data model

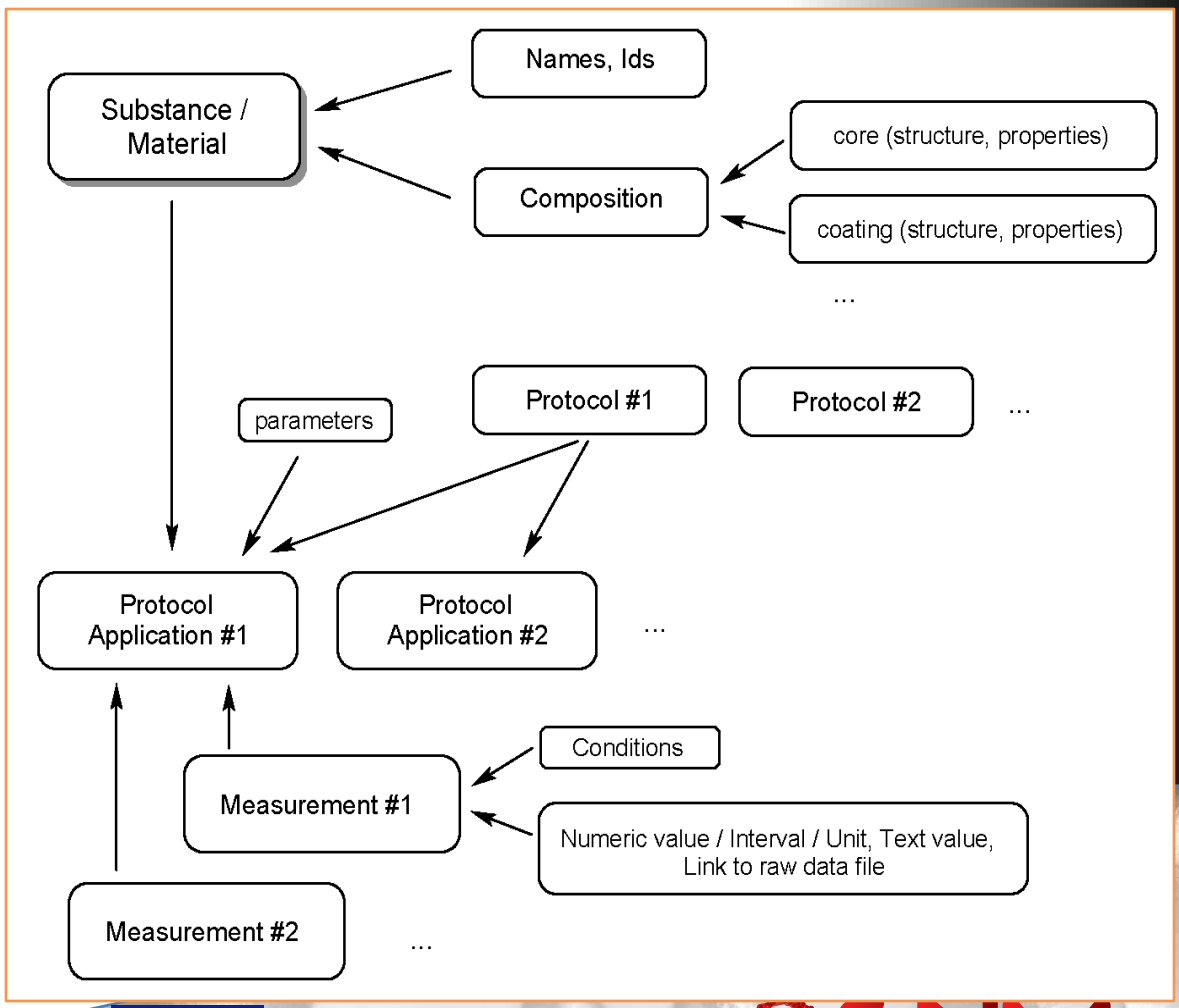
Try it out! Hide Response

Request URL

https://apps.ideaconsult.net:443/enanomapper/substance/IUC5-5f313d1f-4129-499c-abbe-ac

Response Body

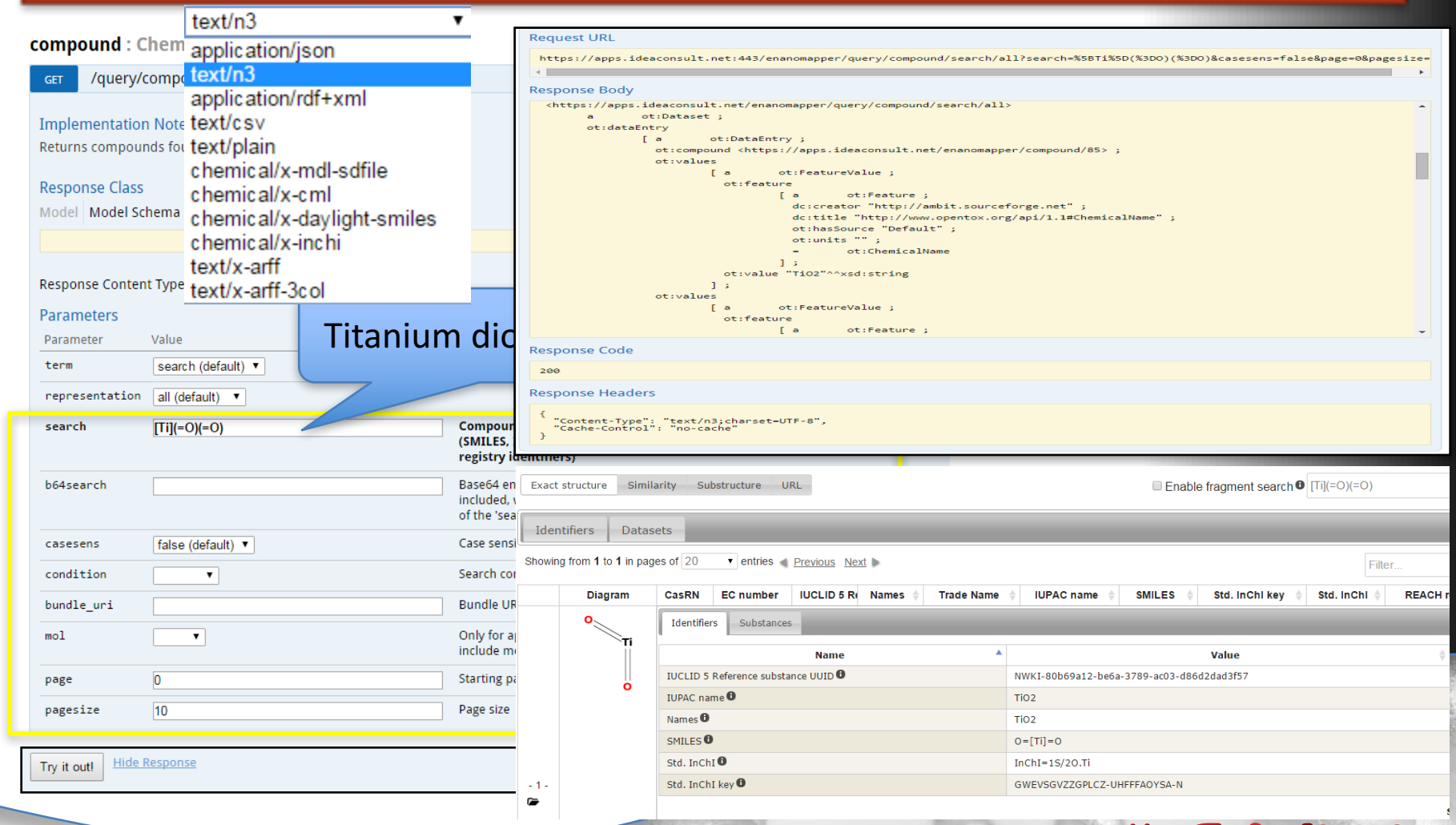

```
"topcategory": "TOX",
"category": {
  "code": "TO_ACUTE_ORAL_SECTION",
  "title": "7.2.1 Acute toxicity - oral"
},
"endpoint": "Acute toxicity: oral.001",
"guideline": [
  "OECD Guideline 423 (Acute Oral toxicity - Acute Toxic Class Method)"
]
},
"parameters": {
  "Sex": "female",
  "Species": "rat"
},
"reliability": {
  "r_isRobustStudy": "false",
  "r_isUsedforClassification": "false",
  "r_isUsedforMSDS": "false",
  "r_purposeFlag": "key study",
  "r_studyResultType": "experimental result",
  "r_value": "1 (reliable without restriction)"
},
"interpretation": {
  "result": "practically nontoxic"
},
"effects": [
  {
    "endpoint": "LDLo",
    "conditions": {
      "Sex": "female"
    },
    "result": {
      "unit": "mg/kg bw",
      "loQualifier": ">=",
      "loValue": 2000
    }
  },
  {
    "endpoint": "LD50 cut-off ",
    "conditions": {
      "Sex": "female"
    },
    "result": {
      "unit": "mg/kg bw",
      "loQualifier": ">=",
      "loValue": 5000
    }
  }
]
```

eNanoMapper

Chemical Structure Search

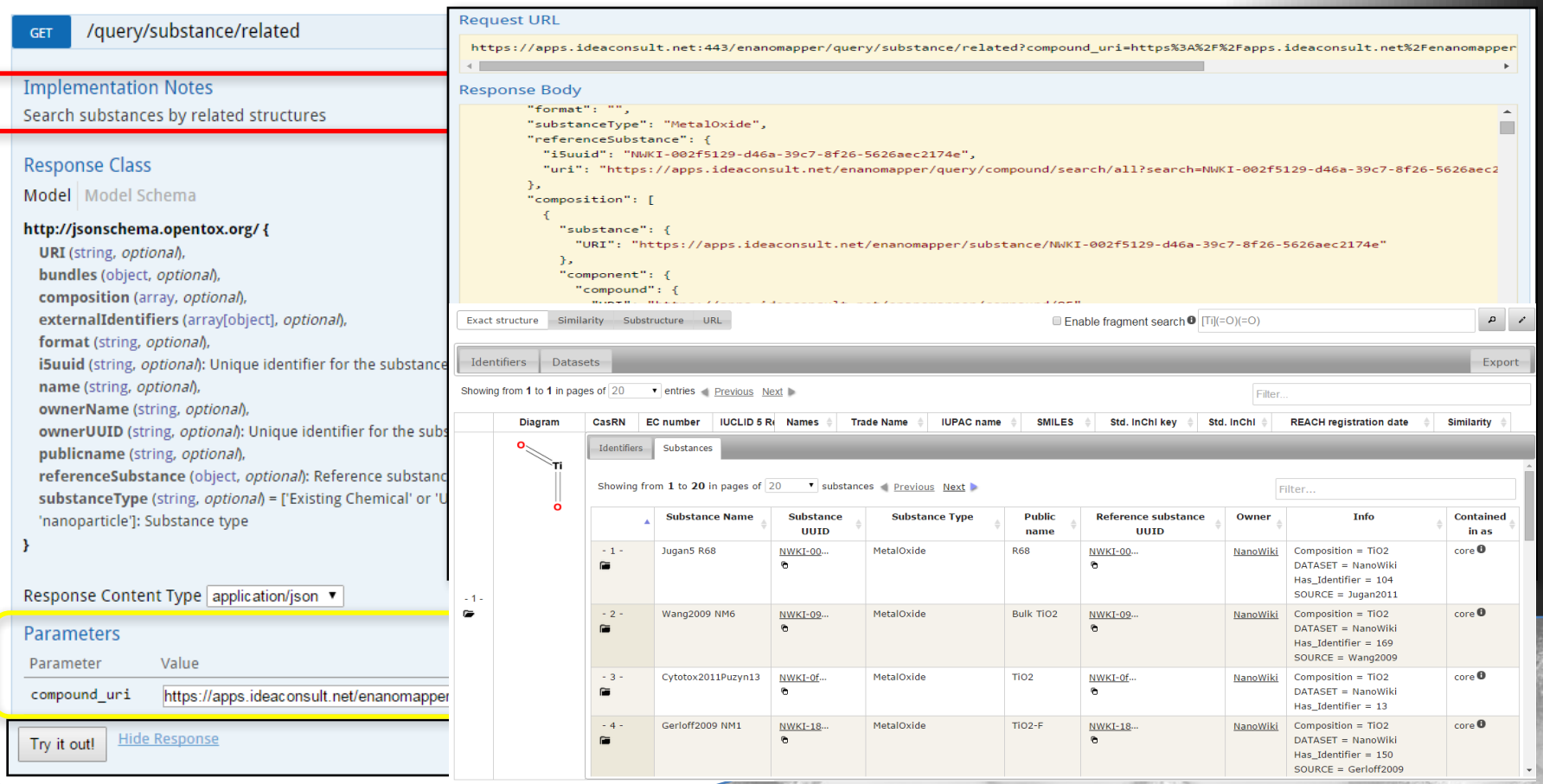
http://enanomapper.github.io/API/#!/compound_0/searchByIdentifier



eNanoMapper

Search nanomaterial by chemical structure

http://enanomapper.github.io/API/#!/substance/searchByRelatedCompound



Nanomaterial components

http://enanomapper.github.io/API/#!/substance_1/getSubstanceComposition

GET /substance/{uuid}/composition

Implementation Notes

Substance composition

Response Class

Model | Model Schema

Response Content Type application/json

Parameters

Request URL

https://apps.ideaconsult.net:443/enanomapper/substance/FCSV-6aea0743-7abb-3448-85ce-961b67fca97f/composition?page=0&pagesize=10

Response Body


```
"component": {
  "compound": {
    "URI": "https://apps.ideaconsult.net/enanomapper/compound/7/conformer/7",
    "structype": "NA",
    "metric": null,
    "name": "",
    "cas": "",
    "einecs": ""
  },
```


uuid

page

pagesi

Try it ou

	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info
- 1 -	G60.AUT	FCSV-6aea0743-7...	nanoparticle	G60.AUT	FCSV-50cca421-d...	Protein Corona Fingerprinting Predicts the Cellular Interaction of Gold and Silver Nanoparticles.csv	Classification = Cationic

Composition name:

Composition UUID: FCSV-6aea0743-7abb-3448-85ce-961b67fca97f

Purity of IUC Substance:

Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges			Structure
Coating	11-Azanylundecane-1-Thiol,Dixrlqjyisysel-Uhfffaoysa-N,Inchi=1s/C11h25ns/C12-10-8-6-4-2-1-3-5-7-9-11-13/H13h,1-12h2,11-Aminoundecane-1-Thiol,11-Amino-1-Undecanethiol			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	
Core	[Au]			0 % (w/w)	0 % (w/w)	0 % (w/w)	Also contained in...	Au

eNanoMapper

Thank you!

Questions?