

Nanomaterial data visualization with ambit.js and d3.js

API Overview

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www.enanomapper.net

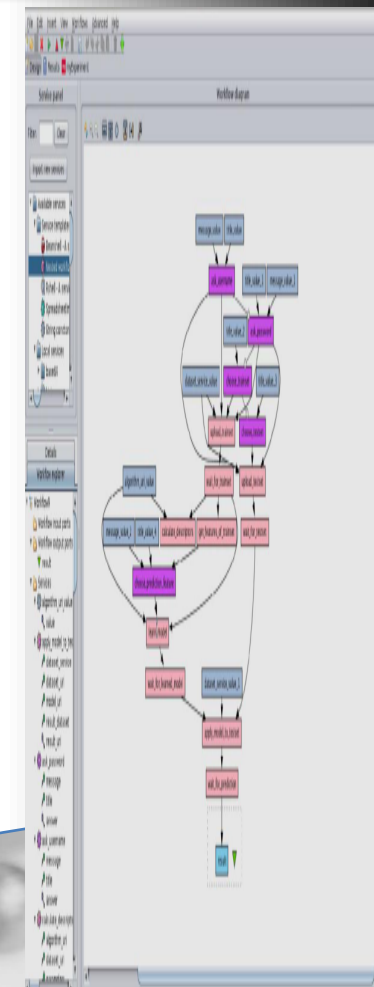
18 May 2015 webinar

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Application Programming Interface (API)

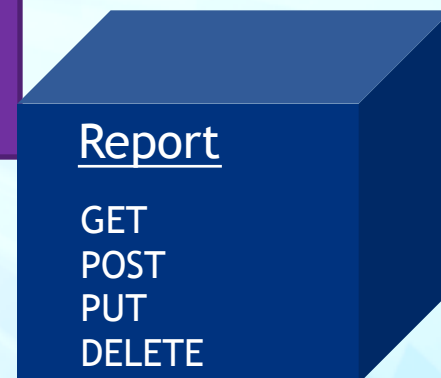
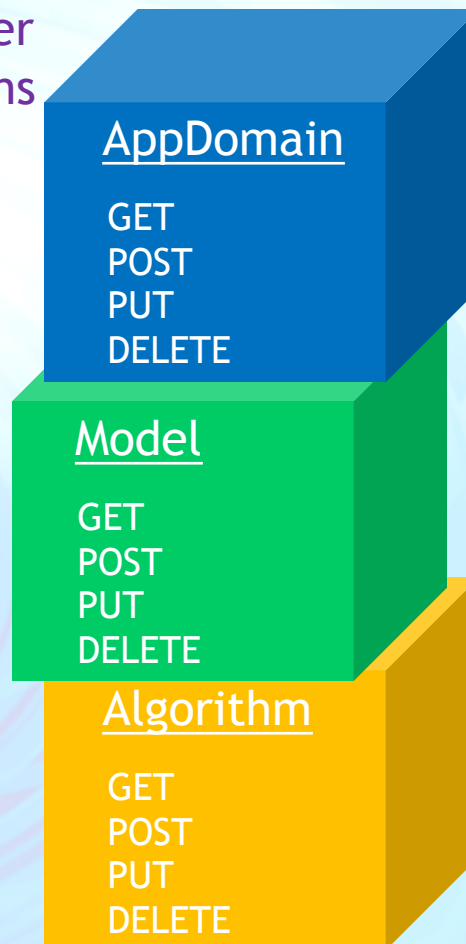
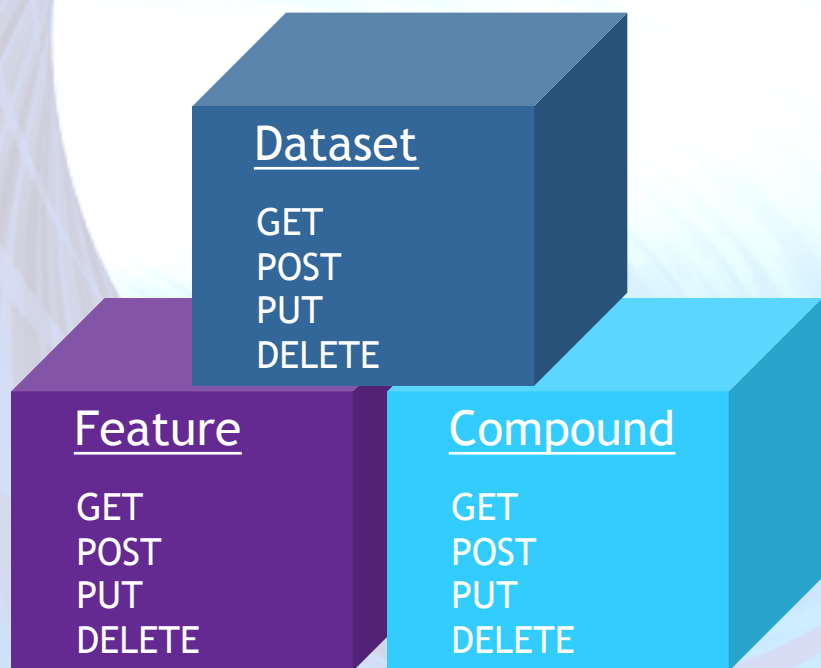
- **API: A way computer programs talk to one another.**
 - *Can be understood in terms of how a programmer sends instructions between programs*
- **The API specifies how software components should interact**
 - *A good API makes it easier to develop a program by providing all the building blocks. A programmer 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)

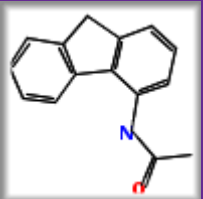
- The way applications talk to each other
- The way developers talk to applications



OpenTox 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	<chem>CN(C)=CC=C(C=C1)N=N/C2=CC=CC=C2C1</chem>	3	3.31	225.3	YES	3.123
http://myhost.com/compound/44497	4-acetamidofluorene	<chem>CC(=O)Nc1ccc2c(c1)ccc3ccccc23</chem>					
...					



```

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.

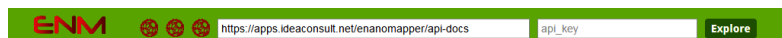
- **Diverse requirements, posed by the nanotechnology community;**
- **Data representation and integration challenges mainly due to data complexity and provenance**
- **Support for data analysis**
 - Requires “spreadsheet” or matrix view of data.
 - The experimental data in the public datasets is usually 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)



eNanoMapper prototype database API

AMBIT REST web services 2.7.2 (with enanomapper profile). More at <https://apps.ideaconsult.net/enanomapper>

[Terms of service](#)
[Contact the developer](#)
[License](#)

algorithm : OpenTox Algorithms service	Show/Hide	List Operations	Expand Operations	Raw
bundle : Datasets of substances	Show/Hide	List Operations	Expand Operations	Raw
compound : OpenTox Chemical Compounds service	Show/Hide	List Operations	Expand Operations	Raw
dataset : OpenTox Dataset service	Show/Hide	List Operations	Expand Operations	Raw
feature : OpenTox Feature service	Show/Hide	List Operations	Expand Operations	Raw
model : OpenTox Prediction Models service	Show/Hide	List Operations	Expand Operations	Raw
property : Chemical substances Properties service	Show/Hide	List Operations	Expand Operations	Raw
query : Queries	Show/Hide	List Operations	Expand Operations	Raw
compound : Chemical structures search	Show/Hide	List Operations	Expand Operations	Raw
substance : Substance search	Show/Hide	List Operations	Expand Operations	Raw
substance : Chemical Substances service	Show/Hide	List Operations	Expand Operations	Raw
GET /substance			List substances	
POST /substance			Import substance(s) and studies	
GET /substance/{uuid}			Get a substance	
GET /substance/{uuid}/composition			Get substance composition	
GET /substance/{uuid}/structures			Get substance composition as a dataset	
GET /substance/{uuid}/study			Get substance study	
GET /substance/{uuid}/studysummary			Get study summary for the substance	
substanceowner : Substance owners	Show/Hide	List Operations	Expand Operations	Raw
task : OpenTox Task service (asynchronous jobs)	Show/Hide	List Operations	Expand Operations	Raw

[BASE URL: <https://apps.ideaconsult.net/enanomapper/api-docs> , API VERSION: 2.7.2]

Interactive API queries

substance : Chemical Substances service

GET /substance

POST /substance

GET /substance/{uuid}

GET /substance/{uuid}/composition

GET /substance/{uuid}/structures

GET /substance/{uuid}/study

Implementation Notes

Substance study

Response Class

Model

Model Schema

```
{
  "interpretation": "object",
  "name": "object",
  "parameters": "object",
  "protocol": "object",
  "reliability": "object",
  "uuid": ""
}
```

Response Content Type: application/json

Parameters

Parameter	Value	Description	Parameter Type	Data Type
uuid	NW1-02981dd4-b7d0-34c8-abab-d817a5a40865	Substance UUID	path	string
top	P-CHEM	Top endpoint category	query	string
category		Endpoint category (the value in the protocol.category code field)	query	string
property		Property UUID	query	string
property_url		Property URI https://apps.ideaconsult.net/enmtest/property/{UUID} - see Property service	query	string
page	0	Starting page	query	int
pageSize	10	Page size	query	int

Response Messages

HTTP Status Code	Reason	Response Model
200	OK	
400	Invalid substance identifier	
404	Substance not found	
403	Forbidden	
401	Not Authorized	
405	Method not allowed	
500	Internal server error	
501	Not implemented	
503	Service unavailable	

Try it out

Hide Response

Request URL

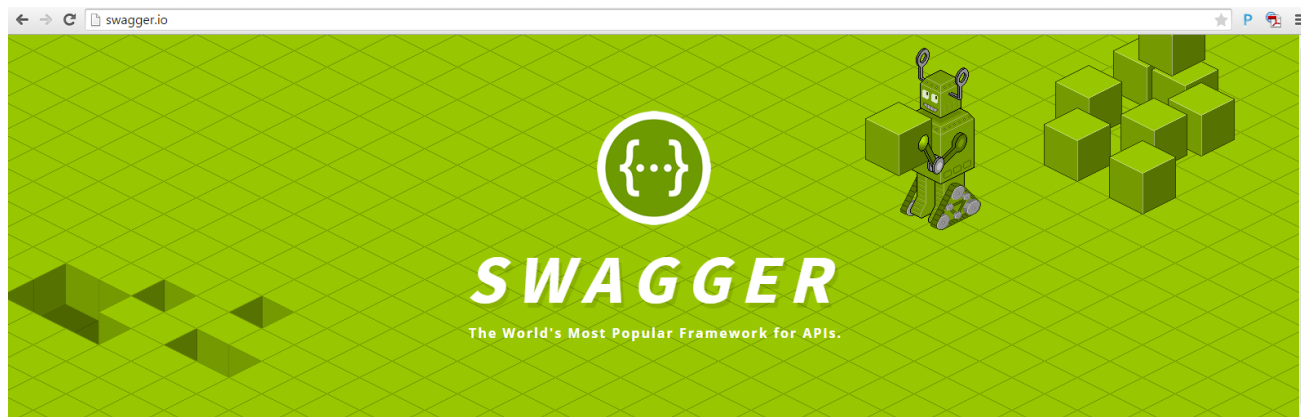
<https://apps.ideaconsult.net:443/enmtest/substance/NW1-02981dd4-b7d0-34c8-abab-d817a5a40865/study?top=P-CHEM&page=0&pageSize=10>

Response Body

```
{
  "TESTPAT_FORM": null,
  "reliability": {
    "isSubstanceStudy": "false",
    "isUsedForClassification": "false",
    "isUsedForForm": "false",
    "purpose": "experimental result",
    "value": null
  },
  "interpretation": {
    "result": null
  },
  "effects": [
    {
      "endpoint": "PARTICLE SIZE",
      "conditions": {},
      "result": {
        "unit": "nm",
        "value": 20
      }
    }
  ]
}
```



API documentation with Swagger



A POWERFUL INTERFACE TO YOUR API

Swagger is a simple yet powerful representation of your RESTful API. With the largest ecosystem of API tooling on the planet, thousands of developers are supporting Swagger in almost every modern programming language. With Swagger, you get interactive documentation, client SDK generation and discoverability.

We created Swagger to help fulfill the promise of APIs. Swagger helps companies like Microsoft, Morningstar, and PayPal build the best possible services with REST APIs.

Now in version 2.0, Swagger is more enabling than ever. And it's 100% open source.

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

"Swagger gives us all the tools we need to build and manage our REST API and documentation. All the details are handled in the toolchain so we can focus on the technical complexities we

Substance search

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

substance : Chemical Substances service

GET /substance

Implementation Notes

Returns a list of substances, according to the search criteria

Response Class

Model | Model Schema

<http://jsonschema.opentox.org/> {

URI (string, optional),
bundles (object, optional),
composition (array, optional),
externalIdentifiers (array(object), optional),
format (string, optional),
I5uuid (string, optional): Unique Identifier for the substance,
name (string, optional),
ownerName (string, optional),
ownerUUID (string, optional): Unique identifier for the substance owner,
publicname (string, optional),
referenceSubstance (object, optional): Reference substance,
substanceType (string, optional) = ['Existing Chemical' or 'UVCB' or 'nanoparticle']: Substance type
}

Response Content Type text/uri-list

Parameters

Parameter	Value
search	"nanotube"
type	like (default)
compound_uri	
bundle_uri	https://apps.ideaconsult.net/enanomapper/bundle/1
page	0
pagesize	10

Try it out! [Hide Response](#)

Request URL

https://apps.ideaconsult.net:443/enanomapper/substance?search=*nanotube*&type=like&bundle_uri=https%3A%2F%2Fapps.ideaconsult.net%2

Response Body

https://apps.ideaconsult.net/enanomapper/substance/IUC5-5f313d1f-4129-499c-abbe-ac18642e2471

Response Code

200

Response Headers

```
{
  "Content-Language": "en",
  "Cache-Control": "private, no-cache",
  "Content-Type": "text/uri-list; charset=UTF-8"
}
```

https://apps.ideaconsult.net/enanomapper/substance?type=like&search=*nanotube*



Search ▾ Nanomaterials ▾ OpenTox ▾ Demo ▾ Help ▾

Search substances by identifiers

Substance search

Name (pattern matching) ▾
"nanotube"
Search

Study: P-Chem ENV ECO TOX

Reliability: 1 2 3 4 5 6

Showing from 1 to 1 in pages of 10 substances ◀ Previous Next ▶

Filter...

	Substance Name	Substance UUID	Substance Type	Public name
- 1 -	Multi-Walled Carbon Nanotubes (MWCNT), synthetic graphite in tubular shape	IUC5-5f313d1f-41...	mono constituent substance	Multi-Walled Carbon Nanotubes (MWCNT), synthetic graphite in tubular shape



Experimental data

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

GET /substance/{uuid}/study

Implementation Notes
Substance study

Response Class
Model | Model Schema

<http://jsonschema.opentox.org/> {
 citation (object, optional),
 effects (array[Effect]),
 interpretation (object, optional),
 owner (object, optional),
 parameters (object, optional),
 protocol (object),
 reliability (object),
 uuid (string): Unique identifier for the study document
}

<http://jsonschema.net/> {
 conditions (object, optional),
 endpoint (string, optional),
 result (Result, optional)
}

<http://jsonschema.opentox.org/> {
 loQualifier (string, optional),
 loValue (number, optional),
 unit (string, optional),
 upQualifier (string, optional),
 upValue (number, optional)
}

Response Content Type

Parameters

Parameter	Value	Description
uuid	IUC5-5f313d1f-4129-499c-abbe-ac18642e2471	Substance UUID
top	P-CHEM	Top endpoint category
category		Endpoint category (field)

[Try it out!](#) [Hide Response](#)

Request URL
<https://apps.ideaconsult.net:443/enanomapper/substance/IUC5-5f313d1f-4129-499c-abbe-ac18642e2471/study?top=P-CHEM&page=0&pagesize=10>

Response Body

```
{
  "effects": [
    {
      "endpoint": "ZETA POTENTIAL",
      "conditions": {
        "MEDIUM": null,
        "Remark": null,
        "STD_DEV": {
          "loValue": 2.9,
          "unit": ""
        },
        "pH": {
          "loValue": "1.9"
        }
      },
      "result": {
        "unit": "mV",
        "loQualifier": "",
        "loValue": 41.4,
        "upQualifier": ""
      }
    }
  ]
}
```

Response Code
200

Response Headers

```
{
  "Content-Type": "application/json; charset=UTF-8",
  "Cache-Control": "no-cache"
}
```

ENM eNanoMapper

Search Nanomaterials OpenTox Demo Help

Substance > IUC5-5f313d1f-4129-499c-abbe-ac18642e2471 > Study

IUC-Substance Composition P-Chem (5) Tox (3)

Filter...

Multi-Walled Carbon Nanotubes (MWCNT), Synthetic Graphite In Tubular Shape

7.2.1 Acute toxicity - oral (1)

Species	Endpoint	Value	Sex	Interpretation of the results	Guideline	Study year	Owner	UUID
rat	LDLo	>= 2000	female	practically nontoxic	OECD Guideline 423 (Acute Oral toxicity - Acute Toxic Class Method)	2006		IUC5-49179f2f-867c-4e7c-8f...
	LD50 cut-off	>= 5000	female					

Showing 1 study(s) (1 to 1)

7.6.1 Genetic toxicity in vitro (1)

Genotoxicity type	Study type	Metabolic activation	Target gene	Species/strain	Metabolic activation	Genotoxicity	Interpretation of the result	Guideline	Study year	Owner	UUID
chromosome and DNA damage	Micronucleus test in vitro (MNvit) and Comet assay in vitro	-	-	A549	without	negative	-		2011		IUC5-6bdaad41-66c2-...
				A549	without	negative					

Showing 1 study(s) (1 to 1)

7.7 Carcinogenicity (1)



Data model

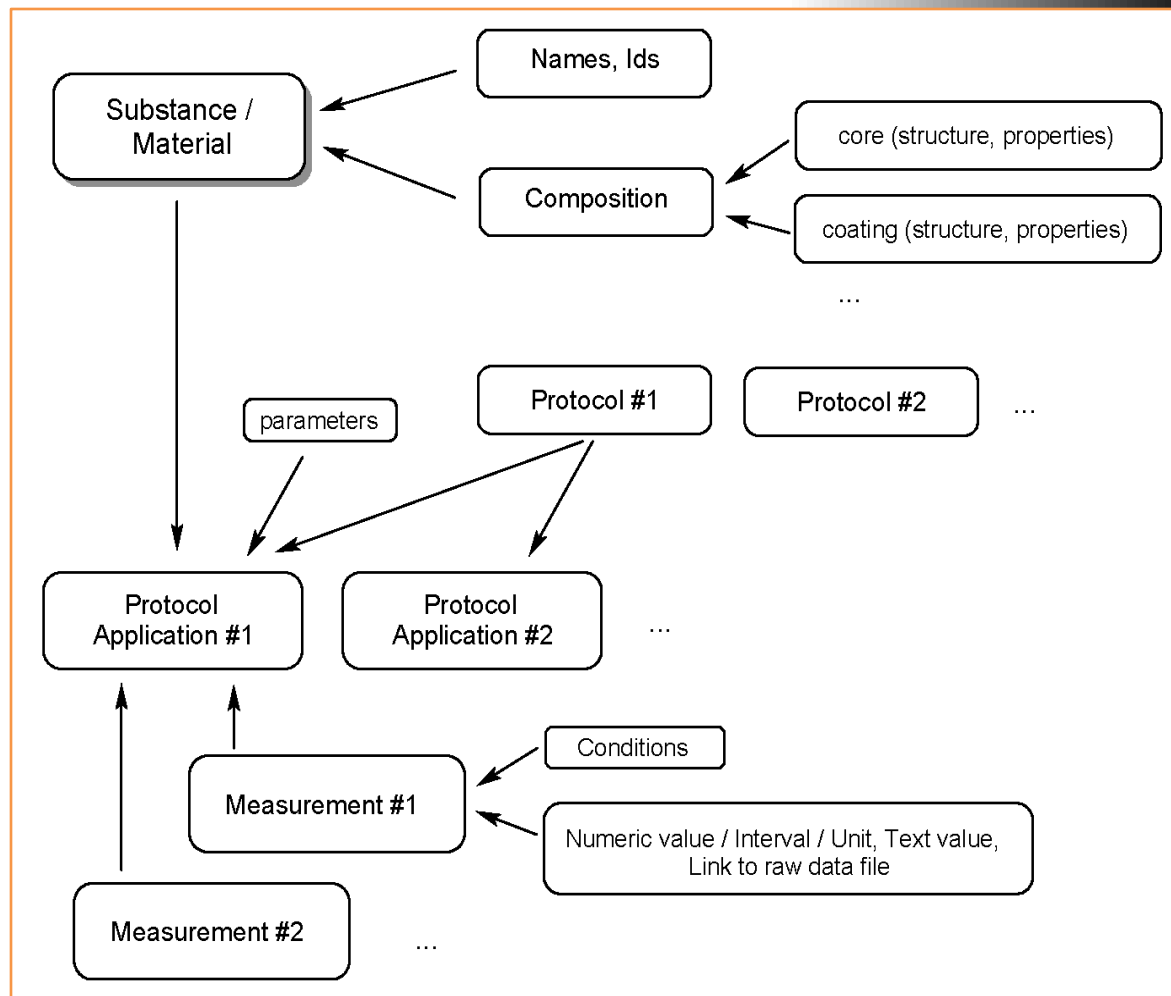
Try it out [Hide Response](#)

Request URL

<https://apps.ideaconsult.net:443/enanomappper/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
      }
    }
  ]
}
```



Chemical Structure Search

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

compound : Chem

GET /query/compound

Implementation Note
Returns compounds for

Response Class
Model | Model Schema

Response Content Type

Parameters

Parameter	Value
term	search (default)
representation	all (default)

search [Ti](=O)(=O) **Titanium dioxide**

b64search

casesens false (default)

condition

bundle_uri

mol

page 0

pagesize 10

Try it out! [Hide Response](#)

Request URL
[https://apps.ideaconsult.net:443/enanomapper/query/compound/search/all?search=%5BTi%5D\(%3DO\)\(%3DO\)&casesens=false&page=0&pagesize=10](https://apps.ideaconsult.net:443/enanomapper/query/compound/search/all?search=%5BTi%5D(%3DO)(%3DO)&casesens=false&page=0&pagesize=10)

Response Body

```
<https://apps.ideaconsult.net/enanomapper/query/compound/search/all>
  a
    ot:Dataset ;
    ot:dataEntry
      [ a
          ot:DataEntry ;
          ot:compound <https://apps.ideaconsult.net/enanomapper/compound/85> ;
          ot:values
            [ a
                ot:FeatureValue ;
                ot:feature
                  [ a
                      ot:Feature ;
                      dc:creator "http://ambit.sourceforge.net" ;
                      dc:title "http://www.opentox.org/api/1.1#ChemicalName" ;
                      ot:hasSource "Default" ;
                      ot:units "" ;
                      -
                        ot:ChemicalName
                      ] ;
                      ot:value "TiO2"^^xsd:string
                    ] ;
                  ot:values
                    [ a
                        ot:FeatureValue ;
                        ot:feature
                          [ a
                              ot:Feature ;
```

Response Code
200

Response Headers

```
{
  "Content-Type": "text/n3;charset=UTF-8",
  "Cache-Control": "no-cache"
}
```

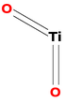
Exact structure Similarity Substructure URL

Enable fragment search [Ti](=O)(=O)

Identifiers Datasets

Showing from 1 to 1 in pages of 20 entries [Previous](#) [Next](#)

Diagram



Identifiers Substances

Name	Value
IUCLID 5 Reference substance UUID	NWKI-80b69a12-be6a-3789-ac03-d86d2dad3f57
IUPAC name	TiO2
Names	TiO2
SMILES	O=[Ti]=O
Std. InChI	InChI=1S/2O.Ti
Std. InChI key	GWEVSGVZZGPLCZ-UHFFFAOYSA-N



Search nanomaterial by chemical structure

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

GET /query/substance/related

Implementation Notes

Search substances by related structures

Response Class

Model [Model Schema](#)

<http://jsonschema.opentox.org/> {

URI (string, optional),
bundles (object, optional),
composition (array, optional),
externalIdentifiers (array[object], optional),
format (string, optional),
iSuuid (string, optional): Unique identifier for the substance
name (string, optional),
ownerName (string, optional),
ownerUUID (string, optional): Unique identifier for the substance
publicname (string, optional),
referenceSubstance (object, optional): Reference substance
substanceType (string, optional) = ['Existing Chemical' or 'U
'nanoparticle']: Substance type

Response Content Type [application/json](#)

Parameters

Parameter Value

compound_uri <https://apps.ideaconsult.net/enanomapper>

Try it out!

[Hide Response](#)

Request URL

https://apps.ideaconsult.net:443/enanomapper/query/substance/related?compound_uri=https%3A%2F%2Fapps.ideaconsult.net%2Fenanomapper


Response Body

```
{
  "format": "",
  "substanceType": "MetalOxide",
  "referenceSubstance": {
    "iSuuid": "NWKI-002f5129-d46a-39c7-8f26-5626aec2174e",
    "uri": "https://apps.ideaconsult.net/enanomapper/query/compound/search/all?search=NWKI-002f5129-d46a-39c7-8f26-5626aec2174e"
  },
  "composition": [
    {
      "substance": {
        "URI": "https://apps.ideaconsult.net/enanomapper/substance/NWKI-002f5129-d46a-39c7-8f26-5626aec2174e"
      },
      "component": {
        "compound": {
          "uri": "https://apps.ideaconsult.net/enanomapper/query/compound/search/all?search=NWKI-002f5129-d46a-39c7-8f26-5626aec2174e"
        }
      }
    }
  ]
}
```

Exact structure Similarity Substructure URL ☐ Enable fragment search [Ti](=O)(=O)

Identifiers Datasets [Export](#)

Showing from 1 to 1 in pages of 20 entries [Previous](#) [Next](#)

Diagram 

Showing from 1 to 20 in pages of 20 substances [Previous](#) [Next](#)

	CasRN	EC number	IUCLID 5 R	Names	Trade Name	IUPAC name	SMILES	Std. InChI key	Std. InChI	REACH registration date	Similarity
Identifiers	Substances										
	Substance Name	Substance UUID	Substance Type	Public name	Reference substance UUID	Owner	Info	Contained in as			
- 1 -	Jugan5 R68	NWKI-00...	MetalOxide	R68	NWKI-00...	NanoWiki	Composition = TiO2 DATASET = NanoWiki Has_Identifier = 104 SOURCE = Jugan2011	core			
- 2 -	Wang2009 NM6	NWKI-02...	MetalOxide	Bulk TiO2	NWKI-02...	NanoWiki	Composition = TiO2 DATASET = NanoWiki Has_Identifier = 169 SOURCE = Wang2009	core			
- 3 -	Cytotox2011Puzyn13	NWKI-0f...	MetalOxide	TiO2	NWKI-0f...	NanoWiki	Composition = TiO2 DATASET = NanoWiki Has_Identifier = 13	core			
- 4 -	Gerloff2009 NM1	NWKI-18...	MetalOxide	TiO2-F	NWKI-18...	NanoWiki	Composition = TiO2 DATASET = NanoWiki Has_Identifier = 150 SOURCE = Gerloff2009	core			



Thank you!

Questions?