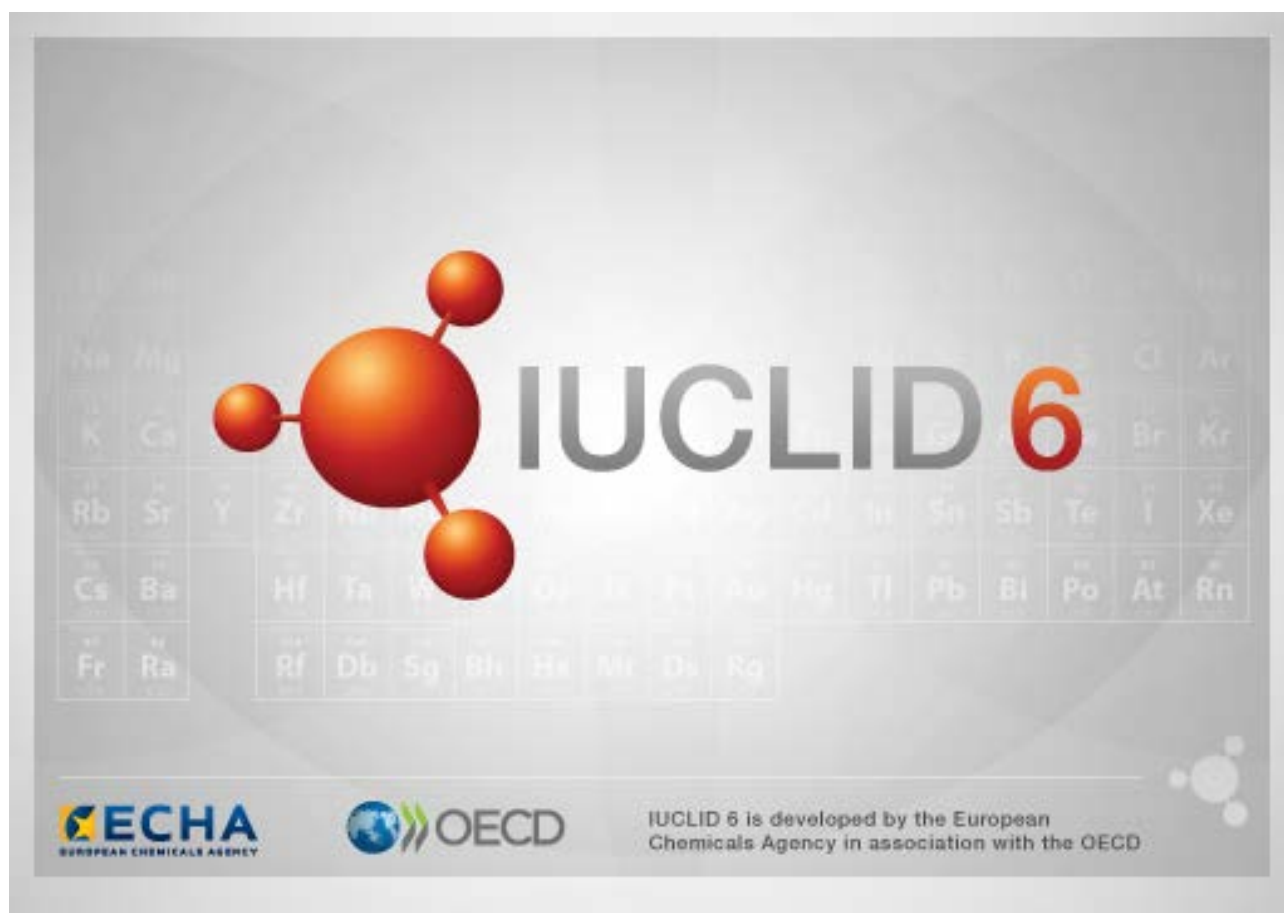


Example use of IUCLID Public REST API for REACH Study Results

16th of August 2021



1. Introduction

This example shows how to extract numerical data about a chemical substance from a Dossier using the IUCLID Public REST API. The starting point for the example is:

Source of Dossiers = REACH Study Results (RSR)

Name of chemical substance = *Formaldehyde*

Section in IUCLID = `ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish`

First, let us clarify some terms and definitions that should make the example clearer.

In IUCLID, data about a chemical substance is stored in a software entity called a Substance. Where the Substance is not in a Dossier, it is often referred to as a *raw* Substance dataset or sometimes just plain Substance dataset. The term *raw* indicates that the Substance is not in a Dossier. When a Dossier is created from a *raw* Substance dataset, a read-only copy of the Substance dataset is copied into the Dossier. A Dossier also contains a header.

RSR contains an aggregated Dossier per REACH registration. For a joint submission under REACH, the aggregated Dossier contains data from all the member Dossiers. In RSR there can be more than one Dossier per chemical substance because there can be individual and joint submissions for the same chemical substance.

2. Identify the Dossier(s) that contain the data of interest

Consider an instance of IUCLID 6 into which the RSR Dossiers of interest have been imported. It can be IUCLID 6 Desktop or, IUCLID 6 Server. First, as a check for later use of the API, find the UUIDs of the Dossiers of interest by some means other than the API. Search for the chemical name *Formaldehyde* either in the interface of IUCLID 6 or, in the index file available on the IUCLID website:

```
reach_study_results-dossier_info_20-08-2020.xlsx
```

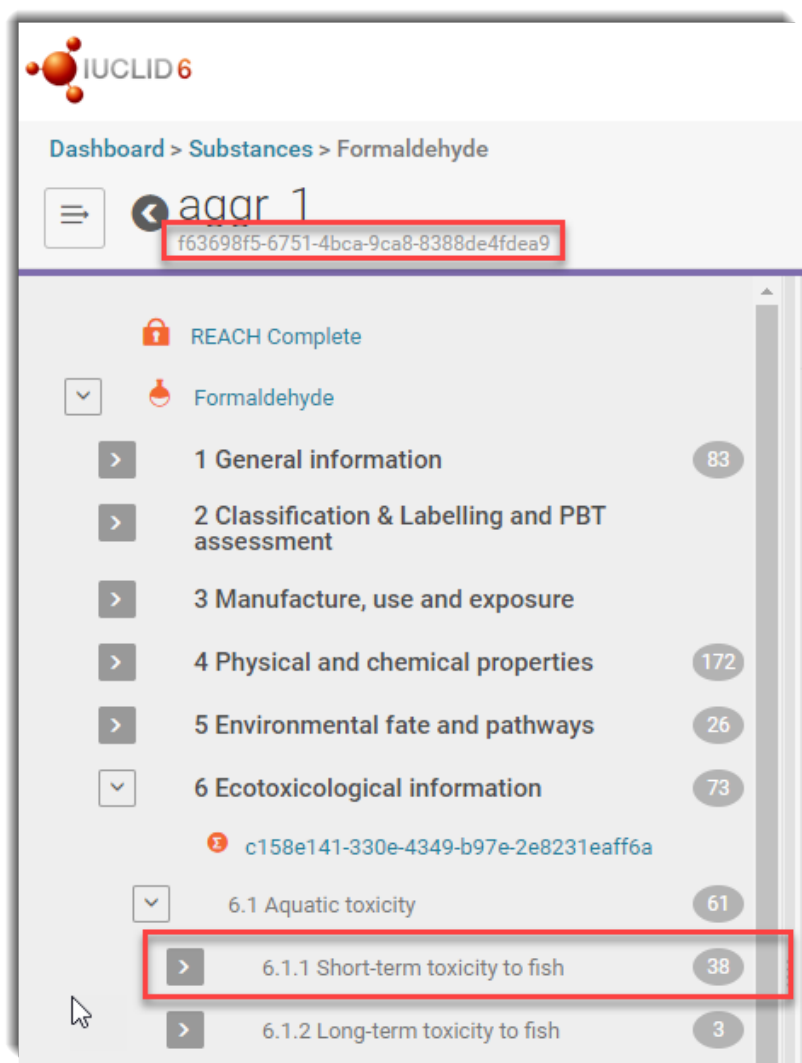
This finds two Dossier UUIDs:

306f1166-e1b1-4300-bade-8f3729c6c638

f63698f5-6751-4bca-9ca8-8388de4fdea9

Check from the IUCLID web interface what data is present in the section `ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish`

The number of ESRs is shown is indicated next to the section, as shown below.



306f1166-e1b1-4300-bade-8f3729c6c638 no data

f63698f5-6751-4bca-9ca8-8388de4fdea9 38 Endpoint study records

Use the API to find the UUIDs of Dossiers that contain a Substance named *Formaldehyde*. The data are obtained using the HTTP GET method. The syntax of the URL used in the method can be broken down into its constituent parts as follows:

Description of part of URI	Part of URI
Base	localhost:8080/iuclid6-ext/api/ext/v1/query/iuclid6/
Type of entity in which to search	bySubstance?
Type of entity to return	doc.type=DOSSIER
Search criterion	&sub.chemical=Formaldehyde

In this example, HTTP requests are made using the application curl on the command line in Git Bash, but you can use the application that suits you best. The data is returned in json format. The data is available for further processing as is, but to view it in a more human readable form, append the following code to the HTTP request command. The system will need to have an installation of python:

```
| python -m json.tool

$ curl -v -X GET "http://localhost:8080/iuclid6-ext/api/ext/v1
/query/iuclid6/bySubstance?doc.type=DOSSIER&sub.chemical=Formaldehyde"
--header "accept: application/vnd.iuclid6.ext+json;
type=iuclid6.Document"
--header "iuclid6-user: SuperUser"
--header "iuclid6-pass: root"
| python -m json.tool
```

The data returned are:

```
{
  "limit" : 10,
  "results" : [
    {
      "representation" : null,
      "uri" : "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9"
    },
    {
      "representation" : null,
      "uri" : "iuclid6:/306f1166-e1b1-4300-bade-8f3729c6c638"
    }
  ],
  "totalCount" : 2
}
```

This agrees with the Dossier UUIDs found via the user interface.

3. Identify the documents that contain the data of interest

The next step is to identify the documents in section `ShortTermToxicityToFish`. The documents are in a Substance that is the *subject* of the Dossier. We know that there is data of interest in a Substance in the Dossier that has UUID of `f63698f5-6751-4bca-9ca8-8388de4fdea9`.

The following command identifies the Substance, and ultimately the documents in section `ShortTermToxicityToFish`. Note that in this example, the optional switch `-v` must be set so that the HTTP headers are displayed. Also, there is no need for the python command.

```
$ curl -v -X GET "http://localhost:8080/iuclid6-ext/api/ext/v1
/dossier/f63698f5-6751-4bca-9ca8-8388de4fdea9
/subject
/document/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish"
--header "accept: application/vnd.iuclid6.ext+json;
type=iuclid6.Document"
--header "iuclid6-user: SuperUser"
--header "iuclid6-pass: root"
```

The response contains a redirect URL that contains the UUID of the Substance dataset in the Dossier. Note that dependent on which software tool you use to make the HTTP request, the redirect may be done automatically, in which case results identifying documents are returned. The `curl` command given above does not make the redirect automatically, so you have to do it yourself. Look for the redirect URI in the header of the HTTP response. Here it is for our example:

```
< HTTP/1.1 308
< Server: Payara Server 4.1.2.174 #badassfish
< Vary: Accept, Accept-Language
< Location: http://localhost:8080/iuclid6-ext/api/ext/v1/dossier/f63698f5-6751-
4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-
3f155510883e/document/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish
< Date: Tue, 24 Nov 2020 14:52:04 GMT
< Content-Length: 0
< X-Frame-Options: SAMEORIGIN
```

The redirect URI replaces the value `/subject/` that was in the original URI, with the type of entity, followed by the UUID of the entity. This means that:

`/subject/`

is replaced by:

`{entity_type}/{entity_uuid}/`

In this example:

`/subject/`

is replaced by:

`/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/`

We now know that the Dossier contains a Substance dataset that has a UUID of:

`e209d92d-959e-447c-a6e3-3f155510883e`.

Therefore, the command to obtain the UUIDs of the next level down in the IUCLID hierarchy, the documents (ESRs) is:

```
$ curl -v -X GET
"http://localhost:8080/iuclid6-ext/api/ext/v1
/dossier/f63698f5-6751-4bca-9ca8-8388de4fdea9
/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e
/document/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish"
--header "iuclid6-user: SuperUser"
--header "iuclid6-pass: root"
| python -m json.tool
```

The results are shown below:

```
{
  "limit": 10,
  "totalCount": 38,
  "results": [
    {
      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/7d2b707d-4b5c-45c3-97a1-aad873c7a8b6",
      "representation": null
    },
    {
      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/a1de0fe6-b0f9-4533-a999-5d9d0f870d11",
      "representation": null
    },
    {
      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/04ea2e73-97d2-4872-a869-da5ed9a17764",
      "representation": null
    },
    {
      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/5201a0ac-27cc-4577-b171-aa045281e027",
      "representation": null
    },
    {
      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/0cedb2a3-0f66-4100-ad1c-d305a9c96f73",
      "representation": null
    },
  ]
}
```

```

      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/4e33727a-45d6-4083-9a97-72fca0d87083",
      "representation": null
    },
    {
      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/5629096c-6bf8-461e-b1d9-3884c8c90bab",
      "representation": null
    },
    {
      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/e2c26fe9-41a9-4c08-9a7f-c66a1b72a1db",
      "representation": null
    },
    {
      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/50f0d1a4-913c-4541-99e4-bf696a464ce1",
      "representation": null
    },
    {
      "uri": "iuclid6:/f63698f5-6751-4bca-9ca8-8388de4fdea9/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish/0f45bf2e-8038-40eb-8b41-77a845958e69",
      "representation": null
    }
  ]
}

```

Each result is a path downwards in the IUCLID hierarchy from the Dossier to an ESR. By default, the output is limited to 10 results. How to set the limits and ranges of output are described in the API documentation on the IUCLID website. To get all the results, increase the limit so that it is equal to the total. The limit is set using an http parameter appended to the URI. The name of the parameter is a lower-case letter "l", as in limit. For example:

```

$ curl -v -X GET
"http://localhost:8080/iuclid6-ext/api/ext/v1
/dossier/f63698f5-6751-4bca-9ca8-8388de4fdea9
/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e
/document/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish?l=38"
--header "iuclid6-user: SuperUser"
--header "iuclid6-pass: root"
| python -m json.tool

```

4. Read the data from a document

There are 38 results in total. This is the correct number of ESRs in the section as viewed from the web interface of IUCLID. The results tell us the UUIDs of the ESRs that contain the numerical data we want to find. To get the actual data from an ESR document, do a query on it.

e.g. for the tenth result, in which the UUID of the ESR is 0f45bf2e-8038-40eb-8b41-77a845958e69.

```
$ curl -v -X GET "http://localhost:8080/iuclid6-ext/api/ext/v1
/dossier/f63698f5-6751-4bca-9ca8-8388de4fdea9
/SUBSTANCE/e209d92d-959e-447c-a6e3-3f155510883e
/document/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish
/0f45bf2e-8038-40eb-8b41-77a845958e69"
--header "accept: application/vnd.iuclid6.ext+json;
type=iuclid6.Document"
--header "iuclid6-user: SuperUser"
--header "iuclid6-pass: root"
| python -m json.tool
```

The data returned is:

```
[
  {
    "key": "0f45bf2e-8038-40eb-8b41-77a845958e69/f63698f5-6751-4bca-9ca8-8388de4fdea9",
    "definition": "ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish",
    "definitionVersion": "5.0",
    "parentKey": "e209d92d-959e-447c-a6e3-3f155510883e/f63698f5-6751-4bca-9ca8-8388de4fdea9",
    "parentDefinition": "SUBSTANCE",
    "parentDefinitionVersion": "5.0",
    "order": 10,
    "createdOn": "2020-08-25T14:05:28Z",
    "modifiedOn": "2017-10-11T05:38:35Z",
    "creationTool": "IUC6"
  },
  {
    "AdministrativeData": {
      "Endpoint": {
        "code": "3335"
      },
      "StudyResultType": {
        "code": "1895"
      },
      "PurposeFlag": {
        "code": "1590"
      },
      "Reliability": {
        "code": "18"
      }
    }
  },
]
```



```
"DataSource": {
  "Reference": [
    "a0d99ace-aae4-4207-ab2d-2717f122436d/f63698f5-6751-4bca-9ca8-8388de4fdea9"
  ],
},
"MaterialsAndMethods": {
  "Guideline": [
    {
      "uuid": "c059e521-5238-4b0a-b3d7-11d9280c9c2d",
      "Qualifier": {
        "code": "2172"
      }
    }
  ],
  "MethodNoGuideline": "No official international or national guideline was followed. Nevertheless, the tests were conducted according to standard procedures.\nLennon RE and Walker CR (1964): Laboratories and methods for screening fish control chemicals . U.S. Fish Wildl Serv Invest Fish Control 1 (Circ No 185) 15 pp \nCommittee on Methods for Toxicity tests with Aquatic Organisms (1975): Methods for acute toxicity tests with fish, macroinvertebrates, and amphibians. Ecological Research Series- EPA (Environ Prot Agency)-660/3-75-009, 61 pp",
  "GLPComplianceStatement": {
    "code": "2158"
  },
  "TestMaterials": {
    "TestMaterialInformation": "3d4d0c17-68f9-4fb0-bd0c-53b469eb1d18/f63698f5-6751-4bca-9ca8-8388de4fdea9"
  },
  "TestOrganisms": {
    "TestOrganismsSpecies": {
      "code": "1319"
    }
  },
  "StudyDesign": {
    "TestType": {
      "code": "1914"
    },
    "WaterMediaType": {
      "code": "1920"
    },
    "LimitTest": {
      "code": "2158"
    },
    "TotalExposureDuration": {
      "value": 96.0,
      "unit": {
        "code": "1976"
      }
    }
  },
  "TestConditions": {
```

```
    "ReferenceSubstancePositiveControl": {
      "code": "2158"
    }
  },
  "ResultsAndDiscussion": {
    "EffectConcentrations": [
      {
        "uuid": "89a9d5e2-b716-4a5f-a01d-d8e8db780b74",
        "KeyResult": false,
        "Duration": {
          "value": 24.0,
          "unit": {
            "code": "1976"
          }
        },
        "Endpoint": {
          "code": "926"
        },
        "EffectConc": {
          "lowerValue": 120.0,
          "unit": {
            "code": "2098"
          }
        },
        "NominalMeasured": {
          "code": "2178"
        },
        "ConcBasedOn": {
          "code": "1754"
        },
        "BasisForEffect": {
          "code": "2135"
        },
        "RemarksOnResults": {
          "code": "1342"
        }
      },
      {
        "uuid": "5113b652-12e7-4cb9-aba7-64ca8fb2a3e2",
        "KeyResult": false,
        "Duration": {
          "value": 96.0,
          "unit": {
            "code": "1976"
          }
        },
        "Endpoint": {
          "code": "926"
        },
        "EffectConc": {
          "lowerValue": 47.15,
          "unit": {
```

```

        "code": "2098"
      }
    },
    "NominalMeasured": {
      "code": "2178"
    },
    "ConcBasedOn": {
      "code": "1754"
    },
    "BasisForEffect": {
      "code": "2135"
    },
    "RemarksOnResults": {
      "code": "1342"
    }
  }
]
},
"ApplicantSummaryAndConclusion": {
  "ValidityCriteriaFulfilled": {
    "code": "2207"
  }
}
}
]

```

This is the data in the single ESR document. To get all the data in the IUCLID section for the Substance, do a query for each of the 38 documents.

An example of numerical data taken from the listing above, highlighted in red, is repeated below for clarity. The data is the first value under *Results and discussion / Effect concentrations* in the 10th ESR.

```

"EffectConc": {
  "lowerValue": 120.0,
  "unit": {
    "code": "2098"
  }
},

```

The meanings of the codes are defined in phrase groups. For example, the values that are available for a field for which there is a multiple picklist are defined in a single phrase group. The phrase group of the field is stated in the definition of the document that contains the field. As described in the documentation of the REST API, the syntax to obtain the definition of a document is:

```
GET /definition/document/{document_type}
```

The type of document is the value of the parameter *definition* in the document. From the output above we can see that:

```
"definition": "ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish",
```

Therefore, in our example, the type of document is:

```
ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish
```

Note that the media type for the document definition must be passed in the following HTTP parameter.

```
application/vnd.iuclid6.ext+json;type=iuclid6.Definition
```

The command to get the definition is:

```
$ curl -v -X GET http://localhost:8080/iuclid6-ext/api/ext/v1
/definition/document/ENDPOINT_STUDY_RECORD.ShortTermToxicityToFish
--header "accept: application/vnd.iuclid6.ext+json;
type=iuclid6.Definition"
--header "iuclid6-user: SuperUser"
--header "iuclid6-pass: root"
| python -m json.tool
```

The relevant part for our example of *EffectConc* is:

```
{
  "type": "range",
  "name": "EffectConc",
  "title": "Effect conc.",
  "multilingual": true,
  "documentSummaryPart": true,
  "tags": [
    "DocumentSummary",
    "ECHA_Dissemination_BriefProfiles_v4.1.1",
    "eChemPortal-PA_v2.0",
    "eChemPortal-PA_v3.0"
  ],
  "numericType": "DOUBLE",
  "unitPhrasegroup": "E05-FishTox",
  "lowerBoundQualifiers": [
    "ca.",
    ">",
    ">="
  ],
  "upperBoundQualifiers": [
    "ca.",
    "<",
    "<="
  ]
},
```

Thus, the phrase group is *E05-FishTox*.

As described in the documentation of the REST API, the syntax to obtain the phrases in a phrase group is:

```
GET /definition/phrasegroup/{phrasegroup-code}/phrases
```

Note that the media type for the document definition does not have to be defined in the HTTP header: The command to get the text values of the phrases that correspond to their codes is:

```
$ curl -v -X GET "http://localhost:8080/iuclid6-ext/api/ext/v1
/definition/phrasegroup/E05-FishTox/phrases"
--header "iuclid6-user: SuperUser"
--header "iuclid6-pass: root"
| python -m json.tool
```

The relevant part for our example of the phrase *2098* in phrase group *E05-FishTox* is:

```
{
  "phrase": {
    "code": "2098",
    "text": "mg/L",
    "description": "",
    "open": false
  },
  "obsolete": false,
  "selectable": true,
  "parentCode": "E05-FishTox"
},
```

Therefore, the effect concentration is *120.0 mg/L*. This can be confirmed from the web interface of IUCLID by navigating to the ESR, and then viewing *Results and discussion*, as shown below.

6.1 Aquatic toxicity (61)

6.1.1 Short-term toxicity to fish (38)

- > 7d2b707d-4b5c-45c3-97a1-aad873c7a8b6
- > a1de0fe6-b0f9-4533-a999-5d9d0f870d11
- > 04ea2e73-97d2-4872-a869-da5ed9a17764
- > 5201a0ac-27cc-4577-b171-aa045281e027
- > 0cedb2a3-0f66-4100-ad1c-d305a9c96f73
- > 4e33727a-45d6-4083-9a97-72fca0d87083
- > 5629096c-6bf8-461e-b1d9-3884c8c90bab
- > e2c26fe9-41a9-4c08-9a7f-c66a1b72a1db
- > 50f0d1a4-913c-4541-99e4-bf696a464ce1
- > 0f45bf2e-8038-40eb-8b41-77a845958e69
- > 86d42299-523a-4df8-8016-20e57731aafe

Results and discussion

Effect concentrations

#..	Key result	Duration	Dose descri...	Effect conc.
1	<input type="checkbox"/> Key result	24 h	LC50	120 mg/L
2	<input type="checkbox"/> Key result	96 h	LC50	47.15 mg/L

Tip

As an alternative to using solely the REST API for determining the structure of IUCLID, or for use in checking the output of the API, you may find it useful to check the IUCLID format directly from the packages available on the [IUCLID website](#). Each package contains an Excel file named IUCLID6_<version>_<date>.xlsx. In that file, the values for phrases are on the sheet named *16Picklists*. The entry for our example is shown below:

A	B	C	D	E
phrasegroup	Phrase group version	Phrase group revision	phraseid	phrasetext
E05-FishTox	v1.0	E05-FishTox - v1.0	116671	CFU/L (mm)
E05-FishTox	v1.0	E05-FishTox - v1.0	116670	CFU/L (nom)
E05-FishTox	v1.0	E05-FishTox - v1.0	116676	IU/L (mm)
E05-FishTox	v1.0	E05-FishTox - v1.0	116677	IU/L (nom)
E05-FishTox	v1.0	E05-FishTox - v1.0	116674	OB/L (mm)
E05-FishTox	v1.0	E05-FishTox - v1.0	116675	OB/L (nom)
E05-FishTox	v1.0	E05-FishTox - v1.0	1935	g/L
E05-FishTox	v1.0	E05-FishTox - v1.0	2098	mg/L
E05-FishTox	v1.0	E05-FishTox - v1.0	2123	mmol/L
E05-FishTox	v1.0	E05-FishTox - v1.0	2127	mol/L
E05-FishTox	v1.0	E05-FishTox - v1.0	2155	ng/L
E05-FishTox	v1.0	E05-FishTox - v1.0	116673	spore/L (mm)
E05-FishTox	v1.0	E05-FishTox - v1.0	116672	spore/L (nom)
E05-FishTox	v1.0	E05-FishTox - v1.0	2500	µg/L
E05-FishTox	v1.0	E05-FishTox - v1.0	2504	µmol/L
E05-FishTox	v1.0	E05-FishTox - v1.0	1342	other:

16Sections | **16Picklists** | 16FreeTextTemplates | Entities | (+)