

Example use of IUCLID Public REST API for REACH Study Results

24th of November 2020



The image displays the IUCLID 6 logo, which consists of a 3D molecular model of a central orange sphere bonded to three smaller orange spheres, positioned to the left of the text "IUCLID 6". The text "IUCLID" is in a grey, sans-serif font, and the number "6" is in a larger, bold, orange font. The background is a faded periodic table of elements.

ECHA
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 **OECD**

IUCLID 6 is developed by the European Chemicals Agency in association with the OECD

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
```

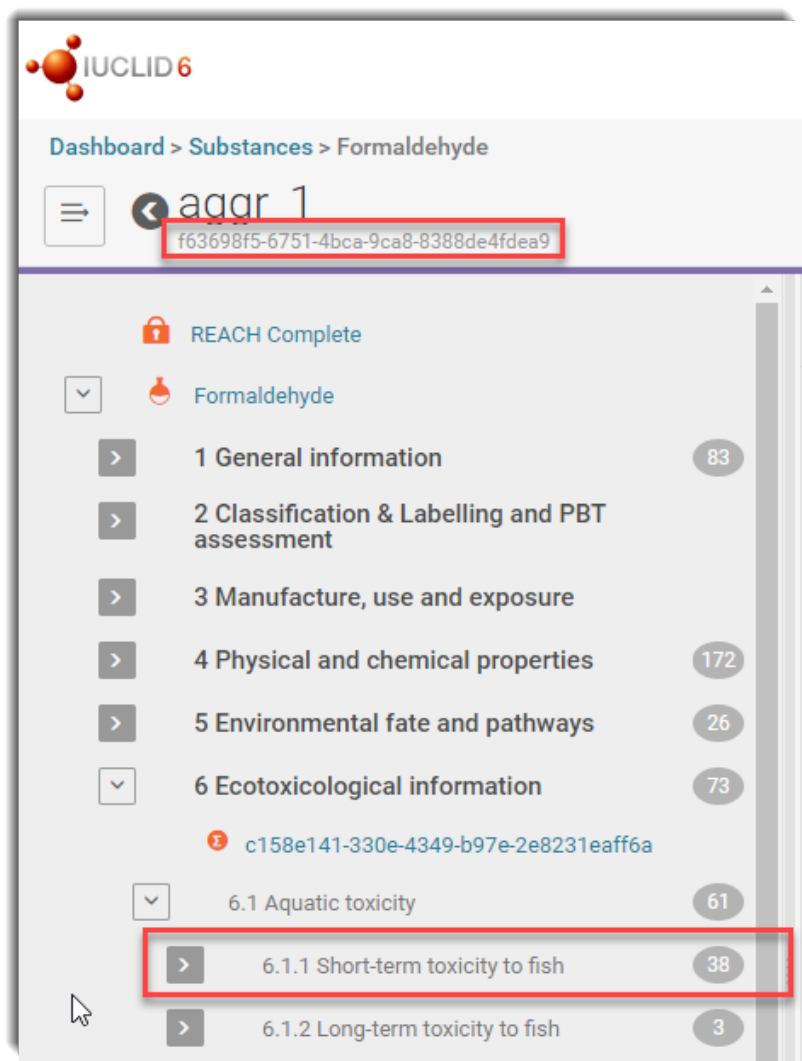
This finds two Dossier UUIDs:

```
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/alde0fe6-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 the IUCLID format for IUCLID 6.4 which is on the [IUCLID website](#). The codes are in the file named `IUCLID6_4_2019-10-28_02-52-18.xlsx`. The values for the numerical fields in this example are on the sheet *I6Picklists*.

Highlighted in red above we can see *Effect concentration* has a lower value of 120.0, and a unit code of 2098 which is mg/L, as shown below:

2763	TD140	v1.0	TD140 - v1.0	2155	ng/L
2764	TD140	v1.0	TD140 - v1.0	2500	µg/L
2765	TD140	v1.0	TD140 - v1.0	2098	mg/L
2766	TD140	v1.0	TD140 - v1.0	1935	g/L
2767	TD110	v1.0	TD110 - v1.0	2154	ng/kg sedim

Ready

Therefore, the effect concentration = 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*.

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