

ICE REST API

- Run ICE Search queries outside of the ICE user interface.
- Data that can be queried include curated in vivo, in vitro, and in silico toxicity data, chemical properties data, and exposure predictions.
- Supported chemical identifiers (ID) include DTXSIDs, CASRNs, InChIKeys, or chemical names.
- Query one chemical ID using GET.
 - Format query as a URL: [https://ice.ntp.niehs.nih.gov/api/v1/search?chemid=\[insert chemical ID\]](https://ice.ntp.niehs.nih.gov/api/v1/search?chemid=[insert chemical ID]).
 - Format query as a URL for Curve Surfer data: [https://ice.ntp.niehs.nih.gov/api/v1/curves?chemid=\[insert chemical ID\]](https://ice.ntp.niehs.nih.gov/api/v1/curves?chemid=[insert chemical ID]).
 - Special characters in a chemical name need to be converted to URL-encode format (https://www.w3schools.com/tags/ref_urlencode.ASP).
 - Results are formatted in JSON.
- Query Curve Surfer data for one single specific biological assay name using GET.
 - Format query as a URL for Curve Surfer Data: [https://ice.ntp.niehs.nih.gov/api/v1/curves?assay=\[insert assay name\]](https://ice.ntp.niehs.nih.gov/api/v1/curves?assay=[insert assay name]).
- Query multiple chemical IDs with specific biological assay or a non-assay endpoint (i.e., chemical property, exposure prediction) or query specific biological assays or a non-assay endpoints for all chemicals using POST.
 - See examples in Slides 2 and 3 of queries built using R and Python code.
 - Results are formatted in JSON: see Slide 4 for result example.
 - Note that the biological assay, non-assay endpoints, and chemical IDs (DTXSID, InChIKeys or chemical names) are **not** case-sensitive in the body of the POST query.



Example R code to query ICE REST API

```
install.packages(c("httr", "jsonlite"));

library("httr");
library("jsonlite");

#Query a single chemical using GET Request
results<-GET("https://ice.ntp.niehs.nih.gov/api/v1/search?chemid=DTXSID7032004")
jsonText<-content(results,"text")
jsonResults<-fromJSON(jsonText)
jsonResults

#Query a list of chemicals using POST Request
bodyContent ='{"chemids": ["YPQLFJODEKMJEF-UHFFFAOYSA-N", "DTXSID8020381", "330-55-2"]}'
results <- POST("https://ice.ntp.niehs.nih.gov/api/v1/search",content_type_json(),body=bodyContent);
jsonText<-content(results,"text")
jsonResults<-fromJSON(jsonText)
jsonResults

#Query a list of specific biological assay and non-assay endpoint for all of the chemicals using POST Request
bodyContent ='{"assays":["Opera, Octanol-Water Distribution Coefficient", "LTea_HepaRG_FAS_up"]} '
results <- POST("https://ice.ntp.niehs.nih.gov/api/v1/search",content_type_json(),body=bodyContent);
jsonText<-content(results,"text")
jsonResults<-fromJSON(jsonText)
jsonResults

#Query a list of chemicals for a specific biological assay and non-assay endpoint using POST Request
bodyContent ='{"chemids": ["YPQLFJODEKMJEF-UHFFFAOYSA-N", "DTXSID8020381", "330-55-2", "Flutamide"], "assays":["Opera, Octanol-Water Distribution Coefficient", "LTea_HepaRG_FAS_up"]} '
results <- POST("https://ice.ntp.niehs.nih.gov/api/v1/search",content_type_json(),body=bodyContent);
jsonText<-content(results,"text")
jsonResults<-fromJSON(jsonText)
jsonResults
```



Example Python code to query ICE REST API

```
pip install requests  
pip install json
```

```
import requests  
import json  
  
#Query a single chemical using GET Request  
response = requests.get("http://ice.ntp.niehs.nih.gov/api/v1/search?chemid=DTXSID7020182")  
print(response);  
json_object = json.loads(response.text)  
print(json.dumps(json_object, indent=4))  
  
#Query a list of chemicals using POST Request  
response = requests.post("http://ice.ntp.niehs.nih.gov/api/v1/search", json={"chemids": ["YPQLFJODEKMJEF-UHFFFAOYSA-N", "DTXSID8020381", "330-55-2", "Flutamide"]})  
print(response);  
json_object = json.loads(response.text)  
print(json.dumps(json_object, indent=1))  
  
#Query a list of specific biological assay and non-assay endpoint for all of the chemicals using POST Request  
response = requests.post("http://ice.ntp.niehs.nih.gov/api/v1/search", json={"assays": ["Opera", "Octanol-Water Distribution Coefficient", "LTea_HepaRG_FAS_up"]})  
print(response);  
json_object = json.loads(response.text)  
print(json.dumps(json_object, indent=1))  
  
#Query a list of chemicals for a specific biological assay and non-assay endpoint using POST Request  
response = requests.post("http://ice.ntp.niehs.nih.gov/api/v1/search", json={"chemids": ["YPQLFJODEKMJEF-UHFFFAOYSA-N", "DTXSID8020381", "330-55-2", "Flutamide"], "assays": ["Opera", "Octanol-Water Distribution Coefficient", "LTea_HepaRG_FAS_up"]})  
print(response);  
json_object = json.loads(response.text)  
print(json.dumps(json_object, indent=1))
```

ICE REST API Results

The screenshot shows a browser window displaying the ICE REST API results for the chemical with ID DTXSID7032004. The URL is https://ice.ntp.niehs.nih.gov/api/v1/search?chemid=DTXSID7032004. The interface includes tabs for 'JSON', 'Raw Data', and 'Headers'. Below the tabs are buttons for 'Save', 'Copy', 'Collapse All', 'Expand All (slow)', and 'Filter JSON'. The main content area displays a JSON object with various properties and their values. The 'assay' key is expanded, showing its value as 'Rat Acute Oral Toxicity'. Other properties include 'endpoint' (LD50), 'substanceType' (Chemical), 'casrn' (13311-84-7), 'qsarReadyId' (MKXXKFYHWDHIYRV-UHFFFAOYSA-N), 'value' (787.0), 'unit' (mg/kg), 'species' (Rat), 'receptorSpecies' (empty string), 'route' (NA), 'sex' (empty string), 'strain' (empty string), 'lifeStage' (empty string), 'tissue' (empty string), 'lesion' (empty string), 'location' (empty string), 'assaySource' (empty string), 'inVitroAssayFormat' (empty string), 'reference' (NLM ChemIDplus TEST (undated)), 'referenceUrl' (https://chem.nlm.nih.gov/chemidplus/), 'dtxsid' (DTXSID7032004), 'substanceName' (Flutamide), and 'pubMedId' (NA). The JSON object continues with other entries (1575-1580) at the bottom.

```
JSON Raw Data Headers
Save Copy Collapse All Expand All (slow) Filter JSON
▶ 1568: ...
▶ 1569: ...
▶ 1570: ...
▶ 1571: ...
▶ 1572: ...
▶ 1573: ...
▼ 1574:
  assay: "Rat Acute Oral Toxicity"
  endpoint: "LD50"
  substanceType: "Chemical"
  casrn: "13311-84-7"
  qsarReadyId: "MKXXKFYHWDHIYRV-UHFFFAOYSA-N"
  value: "787.0"
  unit: "mg/kg"
  species: "Rat"
  receptorSpecies: ""
  route: "NA"
  sex: ""
  strain: ""
  lifeStage: ""
  tissue: ""
  lesion: ""
  location: ""
  assaySource: ""
  inVitroAssayFormat: ""
  reference: "NLM ChemIDplus TEST (undated)"
  referenceUrl: "https://chem.nlm.nih.gov/chemidplus/"
  dtxsid: "DTXSID7032004"
  substanceName: "Flutamide"
  pubMedId: "NA"
▶ 1575: ...
▶ 1576: ...
▶ 1577: ...
▶ 1578: ...
▶ 1579: ...
▼ 1580:
  assay: "NVS_MP_rPBR"
  endpoint: "Top of curve"
  substanceType: "Chemical"
```

- Results are in JSON format as a list of key-value combinations for each chemical queried in the format: key, "value" (for example: assay, "Rat Acute Oral Toxicity"). The "assay" key corresponds to the property name and can be either a biological assay name or the parameter name for a non-assay endpoint (i.e., chemical property, exposure prediction).
- If a biological assay or a chemical parameter is not available in ICE for a queried chemical, then the associated key-value combination will not be returned.
- If a data point is missing, then the relevant key will be returned with a blank value.