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*].
  - Format query as a URL for Curve Surfer data: 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*].
- 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"));
```

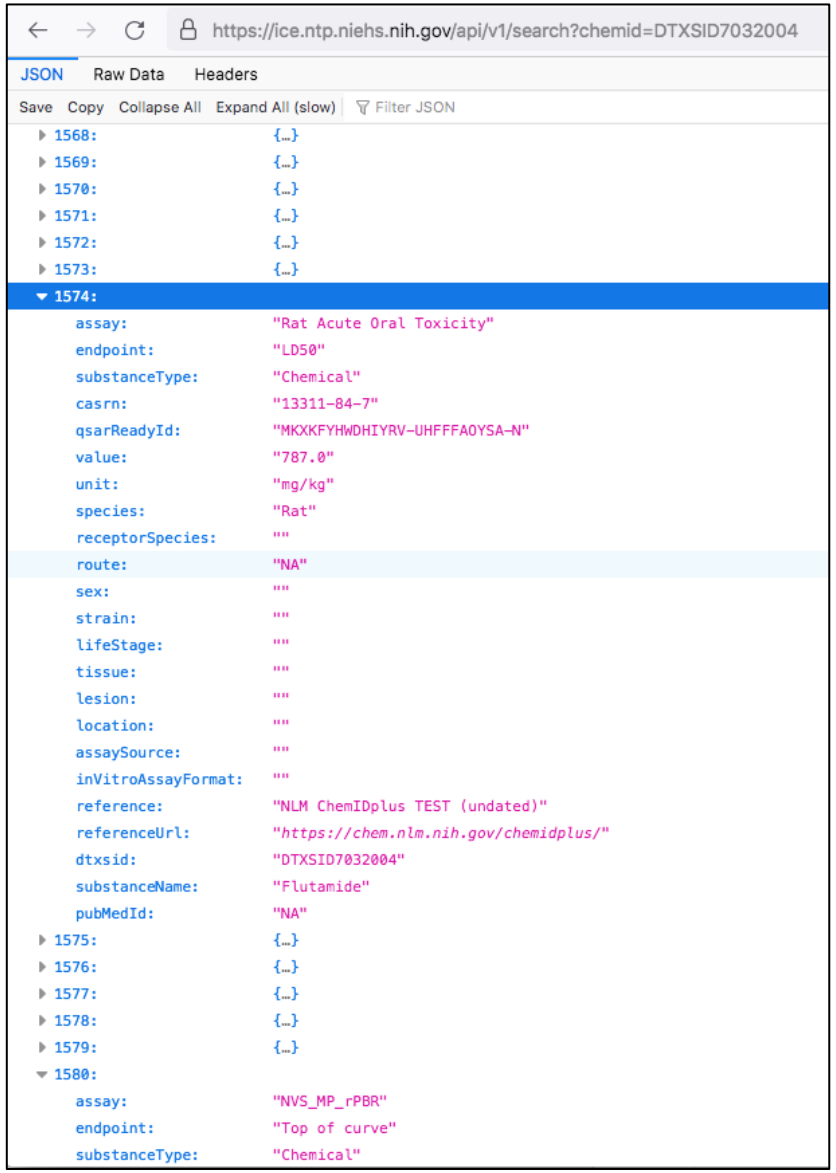
```
library("httr");
library("jsonlite");

#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



- 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.