Open PHACTS
Open Pharmacological Space

Discovery Platform API Walkthrough

Paul Groth
@pgroth
http://www.few.vu.nl/~pgroth/

VU UNIVERSITY AMSTERDAM

- A Simple Restful API
- Registering
- The Hello World of Drug Discovery Apps
- Entry Points
- Compounds
- Targets
- Putting it together
- Going Further

A RESTful API

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Open PHACTS

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OpenPHACTS API Active Docs

The response template for each operation colour coded as follows:

- Required elements that always return a **single value**.
- Required elements that return **either a single value or an array**.
- Optional elements that always return a **single value**
- Optional elements that return **either a single value or an array**.

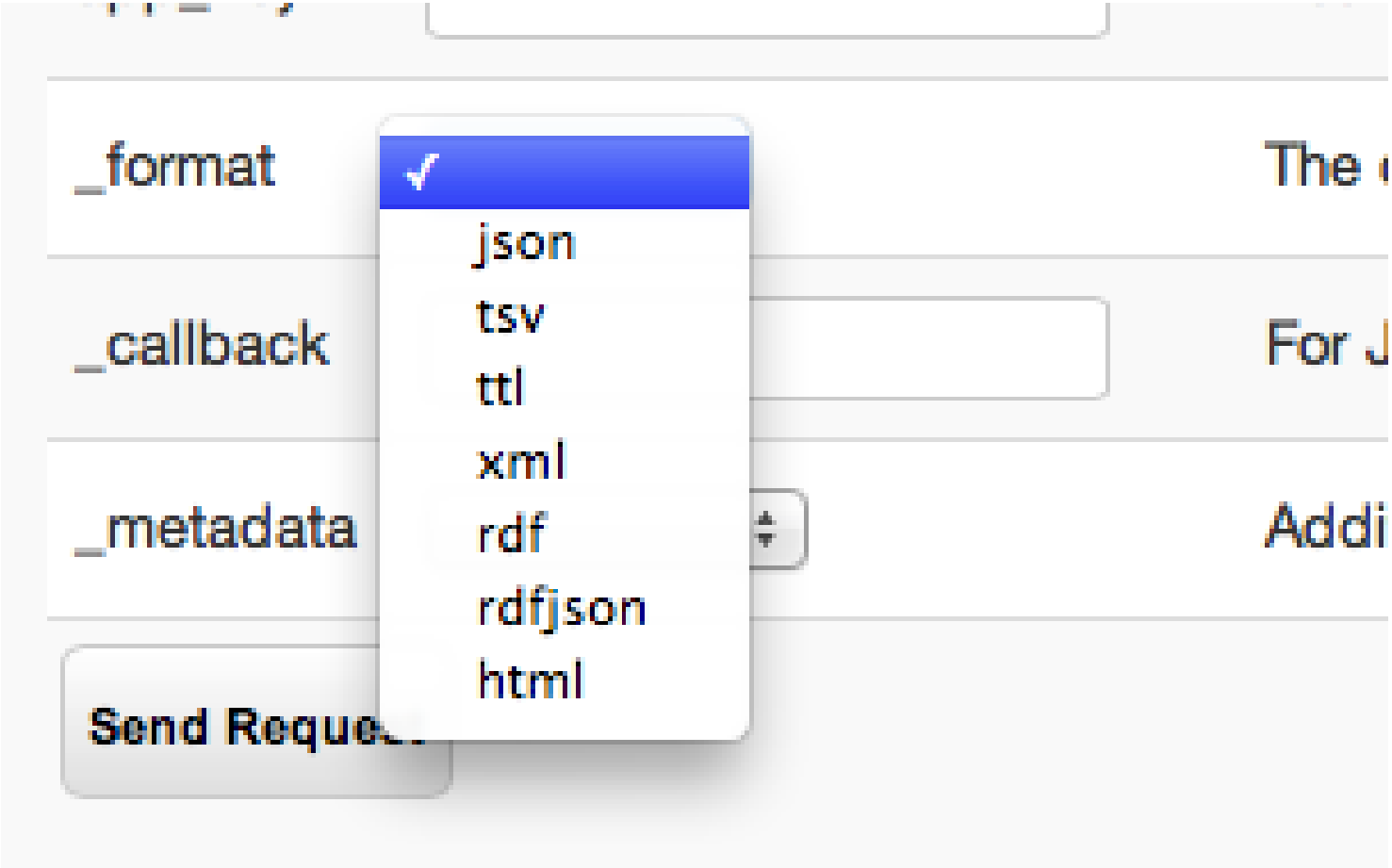
Operations

OpenPHACTS API

Chemical Structure Exact Search	/structure/exact	GET
InchiKey to URL	/structure	GET
Inchi to URL	/structure	GET

Simple http calls for everything (you can put it in a browser)

Supports multiple formats



DEVELOPER & APP KEYS

Open PHACTS

Sign in | Si

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Welcome

Username or Email pgroth@gmail.com

Password

Remember me

Sign in | Sign up | Forgot password?

Application: Open Phacts Demo

For demonstrating the open phacts api

Application ID

This is the application ID, you should send with each API request.

0e939a76

Application Keys

These are application keys used to authenticate requests.

Create new key

1004d9ef5f4ee1ab0bbfc02b623cb955

Properties

State	live
Name	Open Phacts Demo
Description	For demonstrating the open phacts api
Commercial/Non-commercial application	Non-commercial

Edit

Open PHACTS

pgroth Dashboard | Account |

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Application: Open Phacts Demo

For demonstrating the open phacts api

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This is the application ID, you should send with each API request.

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Edit

Dashboard

- Overview
- Applications
- Messages
- Stats

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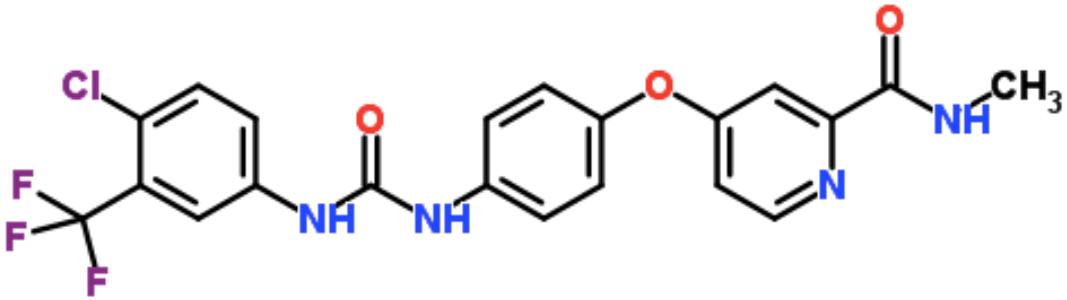
Compound – Target App

Sorafenib



SMILIES:
CNC(=O)c1cc(ccn1)Oc2ccc(cc2)NC(=O)Nc3ccc(c(c3)C(F)(F)F)Cl

ENTRY POINTS

Where do I start?

Open PHACTS
Open Pharmacological Space

The API is URL centric

- http://rdf.chemspider.com/187440
- http://www.conceptwiki.org/concept/38932552-111f-4a4e-a46a-4ed1d7bdf9d5

Where do I start?

Open PHACTS
Open Pharmacological Space

The API is URL centric

- http://rdf.chemspider.com/187440
- http://www.conceptwiki.org/concept/38932552-111f-4a4e-a46a-4ed1d7bdf9d5

Why?

- Ensures precise identification
- Allows for dereferencablity
- Note: supports *many* URLs from different domains

But what if I don't have URL?

Entry Point APIs

Open PHACTS
Open Pharmacological Space

Map free text to a concept URL	/search/freetext	GET
Chemical Structure Exact Search	/structure/exact	GET
InchiKey to URL	/structure	GET
Inchi to URL	/structure	GET
Chemical Structure Similarity Search	/structure/similarity	GET
SMILES to URL	/structure	GET
Chemical Structure Substructure Search	/structure/substructure	GET

Entry Point APIs

Open PHACTS
Open Pharmacological Space

Map free text to a concept URL

/search/freetext GET

Sorafenib

Description

Returns a set of concept URLs associated to the input free text. Driven by ConceptWiki.

PARAMETER	VALUE	DESCRIPTION
app_id	0e939a76	Your access application id
app_key	1004d9ef5f4ee1ab0bbf	Your access application key
q	sorafenib	Query; required. Mininum length is 3 characters. E.g. water
limit		Limits the number of results; optional. Minimum value is 1, maximum value is common sense. Default value is 10.
_format		The desired result format.
_callback		For JSONP
_metadata		Additional metadata to be included with response.

Send Request

HIDE RESPONSE

Entry Point APIs

Open PHACTS
Open Pharmacological Space

Map free text to a concept URL

/search/freetext GET

Description

Returns a set of concept URLs associated to the input free text. Driven by ConceptWiki.

https://beta.openphacts.org/search/freetext?app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&q=sorafenib

app_id	0e939a76	Your access application id
app_key	1004d9ef5f4ee1ab0bbf	Your access application key
q	sorafenib	Query; required. Mininum length is 3 characters. E.g. water
limit		Limits the number of results; optional. Minimum value is 1, maximum value is common sense. Default value is 10.
_format		The desired result format.
_callback		For JSONP
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Send Request HIDE RESPONSE

Entry Point APIs

Open PHACTS
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https://beta.openphacts.org/search/freetext?app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&q=sorafenib

https beta.openphacts.org/search/freetext?app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955 Reader


```
{"format":"linked-data-api","version":"0.2","result":{"_about":"https://beta.openphacts.org/search/freetext?
app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&q=sorafenib","definition":"https://beta.openphacts.org/api-
config","extendedMetadataVersion":"https://beta.openphacts.org/search/freetext?
app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&q=sorafenib&_metadata=all%2Cviews%2Cformats%2Cexecution%2Cbindings%2Cs
ite","primaryTopic":{"result":[{"_about":"http://www.conceptwiki.org/concept/38932552-111f-4a4e-a46a-4ed1d7bdf9d5","match":"
<em>Sorafenib</em>","semanticTag":[{"deleted":false,"uuid":"07a84994-e464-4bbf-812a-a4b96fa3d197","prefLabel_en":"Chemical
Viewed Structurally","prefLabel":"Chemical Viewed Structurally"},{"deleted":false,"uuid":"b6f1866f-4e8c-4674-b1e2-
72f8e2298011","prefLabel_en":"Organic Chemical","prefLabel":"Organic Chemical"}],"altLabel_en":["4-(4-(3-(4-chloro-3-
(trifluoromethyl)phenyl)ureido)phenoxy)-N-methylpicolinamide","BAY-54-9085"," 284461-73-0","Kinome_766","2-pyridinecarboxamide,
4-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenoxy]-N-methyl-","4750207-59-1","4-[4-({[4-chloro-3-
(trifluoromethyl)phenyl]carbamoyl}amino)phenoxy]-N-methylpyridine-2-carboxamide","K00597a","4-(4-(3-(4-chloro-3-
trifluoromethylphenyl)ureido)phenoxy)pyridine-2-carboxyllic acid methyamide","4-[4-({[4-Chloro-3-
(trifluoromethyl)phenyl]carbamoyl}amino)phenoxy]-N-methyl-2-pyridinecarboxamide","sorafenibum","475207-59-1","2-
Pyridinecarboxamide, 4-(4-((((4-chloro-3-(trifluoromethyl)phenyl)amino)carbonyl)amino)phenoxy)-N-methyl-","4-(4-((((4-Chloro-3-
(trifluoromethyl)phenyl)amino)carbonyl)amino)phenoxy)-N-methyl-2-pyridinecarboxamide","BAY 43-9006","N-(4-Chloro-3-
(trifluoromethyl)phenyl)-N'-(4-(2-(N-methylcarbamoyl)-4-pyridyloxy)phenyl)urea","BAY-43-9006","CAS: 284461-73-0","Xarelto","4-
{4-[3-(4-Chloro-3-trifluoromethyl-phenyl)-ureido]-phenoxy}-pyridine-2-carboxylic acid methylamide","284461-73-0","4-{4-[({[4-
CHLORO-3-(TRIFLUOROMETHYL)PHENYL]AMINO}CARBONYL)AMINO]PHENOXY}-N-METHYLPYRIDINE-2-CARBOXAMIDE","BAY-
439006","Nexavar","Sorafenib Tosylate","Sorafenib","4-[4-[[4-Chloro-3-(trifluoromethyl)phenyl]carbamoylamino]phenoxy]-N-methyl-
pyridine-2-carboxamide","BAY-545-9085"],"altLabel":["4-(4-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)phenoxy)-N-
methylpicolinamide","BAY-54-9085"," 284461-73-0","Kinome_766","2-pyridinecarboxamide, 4-[4-[[[[4-chloro-3-
(trifluoromethyl)phenyl]amino]carbonyl]amino]phenoxy]-N-methyl-","4750207-59-1","4-[4-({[4-chloro-3-
(trifluoromethyl)phenyl]carbamoyl}amino)phenoxy]-N-methylpyridine-2-carboxamide","K00597a","4-(4-(3-(4-chloro-3-
trifluoromethylphenyl)ureido)phenoxy)pyridine-2-carboxyllic acid methyamide","4-[4-({[4-Chloro-3-
(trifluoromethyl)phenyl]carbamoyl}amino)phenoxy]-N-methyl-2-pyridinecarboxamide","sorafenibum","475207-59-1","2-
Pyridinecarboxamide, 4-(4-((((4-chloro-3-(trifluoromethyl)phenyl)amino)carbonyl)amino)phenoxy)-N-methyl-","4-(4-((((4-Chloro-3-
(trifluoromethyl)phenyl)amino)carbonyl)amino)phenoxy)-N-methyl-2-pyridinecarboxamide","BAY 43-9006","N-(4-Chloro-3-
(trifluoromethyl)phenyl)-N'-(4-(2-(N-methylcarbamoyl)-4-pyridyloxy)phenyl)urea","BAY-43-9006","CAS: 284461-73-0","Xarelto","4-
{4-[3-(4-Chloro-3-trifluoromethyl-phenyl)-ureido]-phenoxy}-pyridine-2-carboxylic acid methylamide","284461-73-0","4-{4-[({[4-
CHLORO-3-(TRIFLUOROMETHYL)PHENYL]AMINO}CARBONYL)AMINO]PHENOXY}-N-METHYLPYRIDINE-2-CARBOXAMIDE","BAY-
439006","Nexavar","Sorafenib Tosylate","Sorafenib","4-[4-[[4-Chloro-3-(trifluoromethyl)phenyl]carbamoylamino]phenoxy]-N-methyl-
pyridine-2-carboxamide","BAY-545-9085"],"exactMatch":[{"matchType":"ALTERNATIVE","url":"http://www4.wiwiss.fu-
berlin.de/drugbank/resource/drugs/APRD01304"},{"matchType":"ALTERNATIVE","url":"http://purl.uniprot.org/pdb/1uwj"},
{"matchType":"ALTERNATIVE","url":"http://purl.uniprot.org/pdb/1uwh"},
{"matchType":"ALTERNATIVE","url":"http://purl.obolibrary.org/obo/CHEBI_50924"},
{"matchType":"ALTERNATIVE","url":"http://www4.wiwiss.fu-berlin.de/drugbank/resource/drugs/DB00398"},
{"matchType":"ALTERNATIVE","url":"http://www4.wiwiss.fu-berlin.de/drugbank/resource/drugs/216239"},
{"matchType":"PREFERRED","url":"http://purl.bioontology.org/ontology/NCIM/C2713536"},
{"matchType":"ALTERNATIVE","url":"http://purl.uniprot.org/pdb/BAX"},
```

Entry Point APIs

Open PHACTS
Open Pharmacological Space

Response Body


```
{
 "format": "linked-data-api",
 "version": "0.2",
 "result": {
  "_about": "https://beta.openphacts.org/search/freetext?
app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&q=sorafenib",
  "definition": "https://beta.openphacts.org/api-config",
  "extendedMetadataVersion": "https://beta.openphacts.org/search/freetext?
app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&q=sorafenib&_metadata=all%2Cviews%2C
formats%2Cexecution%2Cbindings%2Csite",
  "primaryTopic": {
   "result": [
    {
     "_about": "http://www.conceptwiki.org/concept/38932552-111f-4a4e-a46a-4ed1d7bdf9d5",
     "match": "Sorafenib",
     "semanticTag": [
      {
       "deleted": false,
       "uuid": "07a84994-e464-4bbf-812a-a4b96fa3d197",
       "prefLabel_en": "Chemical Viewed Structurally",
       "prefLabel": "Chemical Viewed Structurally"
      },
      {
       "deleted": false,
       "uuid": "b6f1866f-4e8c-4674-b1e2-72f8e2298011",
```


"_about": "http://www.conceptwiki.org/concept/38932552-111f-4a4e-a46a-4ed1d7bdf9d5"

Entry Point APIs

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SMILES to URL

/structure GET

Description

Returns a ChemSpider URL corresponding to an input SMILES string. Driven by ChemSpider.

CNC(=O)c1cc(ccn1)Oc2ccc(cc2)NC(=O)Nc3ccc(c(c3)C(F)(F)F)Cl

Response template:

?primaryTopic chemspider:smiles ?smiles

PARAMETER	VALUE	DESCRIPTION
app_id	0e939a76	Your access application id
app_key	1004d9ef5f4ee1ab0bbf	Your access application key
smiles	**CNC(=O)c1cc(ccn1)Oc2**	A SMILES string. E.g. CC(=O)Oc1ccccc1C(=O)O
_format		The desired result format.
_callback		For JSONP
_metadata		Additional metadata to be included with response.

Send Request HIDE RESPONSE

Entry Point APIs

Open PHACTS
Open Pharmacological Space

Response Body


```
{
 "format": "linked-data-api",
 "version": "0.2",
 "result": {
  "_about": "https://beta.openphacts.org/structure?
app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&smiles=CNC(%3DO)c1cc(ccn1)Oc2ccc(cc2)NC
(%3DO)Nc3ccc(c(c3)C(F)(F)F)Cl",
  "definition": "https://beta.openphacts.org/api-config",
  "extendedMetadataVersion": "https://beta.openphacts.org/structure?
app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&smiles=CNC(%3DO)c1cc(ccn1)Oc2ccc(cc2)NC
(%3DO)Nc3ccc(c(c3)C(F)(F)F)Cl&_metadata=all%2Cviews%2Cformats%2Cexecution%2Cbindings%2Csite",
  "primaryTopic": {
   "_about": "http://rdf.chemspider.com/187440",
   "smiles": "CNC(=O)c1cc(ccn1)Oc2ccc(cc2)NC(=O)Nc3ccc(c(c3)C(F)(F)F)Cl",
   "isPrimaryTopicOf": "https://beta.openphacts.org/structure?
app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&smiles=CNC(%3DO)c1cc(ccn1)Oc2ccc(cc2)NC
(%3DO)Nc3ccc(c(c3)C(F)(F)F)Cl"
  }
 }
}
```


"_about": "http://rdf.chemspider.com/187440"

COMPOUND APIS

Compound APIs

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Compound Information	/compound	GET
Compound Pharmacology Count	/compound/pharmacology/count	GET
Compound Pharmacology Complete (DEPRECATED)	/compound/pharmacology	GET
Compound Pharmacology Paginated	/compound/pharmacology/pages	GET

Compound APIs: Compound Information

Open PHACTS
Open Pharmacological Space

PARAMETER	VALUE	DESCRIPTION
uri	http://www.conceptwik	A compound URI. e.g.: http://www.conceptwiki.org/concept/38932552-111f-4a4e-a46a-4ed1d7bdf9d5
app_id	0e939a76	Your access application id
app_key	1004d9ef5f4ee1ab0bbf	Your access application key
_format		The desired result format.
_callback		For JSONP
_metadata		Additional metadata to be included with response.

Send Request HIDE RESPONSE

We can use either:
http://www.conceptwiki.org/concept/38932552-111f-4a4e-a46a-4ed1d7bdf9d5
http://rdf.chemspider.com/187440

Compound APIs

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Chembl


```
http://www.conceptwiki.org/concept/38932552-1111-4a4e-a40a-4e010bd19d3",
{
 "_about": "http://data.kasabi.com/dataset/chembl-rdf/chemblid/CHEMBL1336",
 "full_mwt": 464.825,
 "molform": "C21H16ClF3N4O3",
 "mw_freebase": 464.825,
 "rtb": 6,
 "inDataset": "http://data.kasabi.com/dataset/chembl-rdf"
},
{
```


Chemspider


```
  },
  {
   "_about": "http://rdf.chemspider.com/187440",
   "inchi": "InChI=1S/C21H16ClF3N4O3/c1-26-19(30)18-11-15(8-9-27-18)32-14-5-2-12(3-6-14)28-
20(31)29-13-4-7-17(22)16(10-13)21(23,24)25/h2-11H,1H3,(H,26,30)(H2,28,29,31)",
   "inchikey": "MLDQJTXFUGDVEO-UHFFFAOYSA-N",
   "smiles": "CNC(=O)c1cc(ccn1)Oc2ccc(cc2)NC(=O)Nc3ccc(c(c3)C(F)(F)F)Cl",
   "inDataset": "http://www.chemspider.com",
   "hba": 7,
   "hbd": 3,
   "logp": 4.818,
   "psa": 9.235e-18,
   "ro5_violations": 0
  },
```

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Drugbank

provenance - inDataset property


```
    },
    {
    "_about": "http://www4.wiwiss.fu-berlin.de/drugbank/resource/drugs/DB00398",
    "inDataset": "http://linkedlifedata.com/resource/drugbank",
    "biotransformation": "Sorafenib is metabolized primarily in the liver, undergoing
oxidative metabolism, mediated by CYP3A4, as well as glucuronidation mediated by UGT1A9.
Sorafenib accounts for approximately 70-85% of the circulating analytes in plasma at steady-
state. Eight metabolites of sorafenib have been identified, of which five have been detected
in plasma. The main circulating metabolite of sorafenib in plasma, the pyridine N-oxide,
shows in vitro potency similar to that of sorafenib. This metabolite comprises approximately
9-16% of circulating analytes at steady-state.",
    "description": "Sorafenib (rINN), marketed as Nexavar by Bayer, is a drug approved for
the treatment of advanced renal cell carcinoma (primary kidney cancer). It has also received
\"Fast Track\" designation by the FDA for the treatment of advanced hepatocellular carcinoma
(primary liver cancer), and has since performed well in Phase III trials.\nSorafenib is a
small molecular inhibitor of Raf kinase, PDGF (platelet-derived growth factor), VEGF receptor
2 & 3 kinases and c Kit the receptor for Stem cell factor. A growing number of drugs target
most of these pathways. The originality of Sorafenib lays in its simultaneous targeting of
the Raf/Mek/Erk pathway.",
    "proteinBinding": "99.5%",
    "toxicity": "The highest dose of sorafenib studied clinically is 800 mg twice daily. The
adverse reactions observed at this dose were primarily diarrhea and dermatologic events. No
information is available on symptoms of acute overdose in animals because of the saturation
of absorption in oral acute toxicity studies conducted in animals."
    }
```

Compound APIs
Compound Pharmacology Paginated

Open PHACTS
Open Pharmacological Space

PARAMETER	VALUE	DESCRIPTION
uri	**http://rdf.chemspider.c**	A compound URI. e.g.: http://www.conceptwiki.org/concept/38932552-111f-4a4e-a46a-4ed1d7bdf9d5
app_id	0e939a76	Your access application id
app_key	1004d9ef5f4ee1ab0bbf	Your access application key
assay_organism		A literal organism in ChEMBL.
target_organism		A literal target organism in ChEMBL.
activity_type		One of the activity types listed at /pharmacology/filters/activities
activity_value		Return activity values equal to this number.
min-activity_value		Return activity values greater than or equal to this number.
minEx-activity_value		Return activity values greater than this number.
max-activity_value		Return activity values less than or equal to this number.

Compound APIs
Compound Pharmacology Paginated

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		e.g. IC50: /pharmacology/filters/units/IC50
_page	2	A number; the page that should be viewed
_pageSize	10	The desired page size. Set to all to retrieve all results in a single page.


```
{
 "format": "linked-data-api",
 "version": "0.2",
 "result": {
  "_about": "https://beta.openphacts.org/compound/pharmacology/pages?
uri=http%3A%2F%2Frdf.chemspider.com%2F187440&app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b
623cb955&_pageSize=10&_page=2",
  "itemsPerPage": 10,
  "startIndex": 10,
  "isPartOf": {
   "_about": "https://beta.openphacts.org/compound/pharmacology/pages?
uri=http%3A%2F%2Frdf.chemspider.com%2F187440&app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b
623cb955&_pageSize=10",
   "hasPart": "https://beta.openphacts.org/compound/pharmacology/pages?
uri=http%3A%2F%2Frdf.chemspider.com%2F187440&app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b
623cb955&_pageSize=10&_page=2",
   "definition": "http://www.openphacts.org/api#compoundPharmacologyListEndpoint",
   "type": "http://purl.org/linked-data/api/vocab#List"
  },
```

Compound APIs
Compound Pharmacology Paginated

Open PHACTS
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```
"items": [
  {
   "_about": "http://data.kasabi.com/dataset/chembl-rdf/activity/a1650069",
   "pmid": "15711537",
   "forMolecule": {…},
   "onAssay": {
      …
    "target": {
     "_about": "http://data.kasabi.com/dataset/chembl-rdf/chemblid/CHEMBL4226",
     "title": "Dual specificity protein kinase CLK3",
     "organism": "Homo sapiens"
    },
   …
  },
…
]
```

Compound APIs
Compound Pharmacology Paginated

Open PHACTS
Open Pharmacological Space


```
  },
  "onAssay": {
   "_about": "http://data.kasabi.com/dataset/chembl-rdf/chemblid/CHEMBL860651",
   "description": "Average Binding Constant for MKNK2 ; NA=Not Active at 10 uM",
   "target": {
    "_about": "http://data.kasabi.com/dataset/chembl-rdf/chemblid/CHEMBL4204",
    "title": "MAP kinase signal-integrating kinase 2",
    "organism": "Homo sapiens"
   },
   "inDataset": "http://data.kasabi.com/dataset/chembl-rdf",
   "organism": "Homo sapiens"
  },
  "relation": "=",
  "standardUnits": "nM",
  "standardValue": 250,
  "activity_type": "Kd",
  "inDataset": "http://data.kasabi.com/dataset/chembl-rdf"
 },
```

TARGET APIS

Target APIs

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Target Information	/target	GET
Target Pharmacology Count	/target/pharmacology/count	GET
Target Pharmacology Complete (DEPRECATED)	/target/pharmacology	GET
Target Pharmacology Paginated	/target/pharmacology/pages	GET

Target APIs
Target Information

Open PHACTS
Open Pharmacological Space

PARAMETER	VALUE	DESCRIPTION
uri	http://data.kasabi.com/	A target URI. e.g.: http://www.conceptwiki.org/concept/00059958-a045-4581-9dc5-e5a08bb0c291
app_id	0e939a76	Your access application id
app_key	1004d9ef5f4ee1ab0bbf	Your access application key
_format		The desired result format.
_callback		For JSONP
_metadata		Additional metadata to be included with response.

Send Request HIDE RESPONSE

http://data.kasabi.com/dataset/chembl-rdf/chemblid/CHEMBL4226

Target APIs
Target Information


```
      "http://purl.uniprot.org/keywords/963",
      "http://purl.uniprot.org/keywords/539"
     ],
     "existence": "http://purl.uniprot.org/core/Evidence_at_Protein_Level_Existence",
     "organism": "http://purl.uniprot.org/taxonomy/9606",
     "sequence":
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RSSRSVEDDKEGHLVCRIGDWLQERYEIVGNLGEGTFGKVVECLDHARGKSQVALKIIRNVGKYREAARLEINVLKKIKEKDKENKFLCVLMS
DWFNFHGHMCIAFELLGKNTFEFLKENNFQPYPLPHVRHMAYQLCHALRFLHENQLTHTDLKPENILFVNSEFETLYNEHKSCEEKSVKNTSI
RVADFGSATFDHEHHTTIVATRHYRPPEVILELGWAQPCDVWSIGCILFEYYRGFTLFQTHENREHLVMMEKILGPIPSHMIHRTRKQKYFYK
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     "inDataset": "http://purl.uniprot.org",
     "seeAlso": [
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      "http://purl.uniprot.org/pdb/2WU6",
      "http://purl.uniprot.org/pdb/3RAW",
      "http://purl.uniprot.org/pdb/2EU9",
      "http://purl.uniprot.org/pdb/2EXE"
     ]
    },
    "http://data.kasabi.com/dataset/chembl-rdf/chemblid/CHEMBL4226",
    {
     "_about": "http://www.conceptwiki.org/concept/6a05400c-8a68-4a22-b06f-330713d09d81",
     "inDataset": "http://www.conceptwiki.org",
     "prefLabel_en": "CLK3 (Homo sapiens)",
     "prefLabel": "CLK3 (Homo sapiens)"
    },
    {
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PUTTING IT TOGETHER

Compound -> Target in 3 URLs

Open PHACTS
Open Pharmacological Space

1. Keyword to a compound URL

https://beta.openphacts.org/search/freetext?app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&**q=sorafenib**

1. Pharmacology for a compound

https://beta.openphacts.org/compound/pharmacology/pages?**uri=http%3A%2F%2Fwww.conceptwiki.org%2Fconcept%2F38932552-111f-4a4e-a46a-4ed1d7bdf9d5**&app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955&_pageSize=10

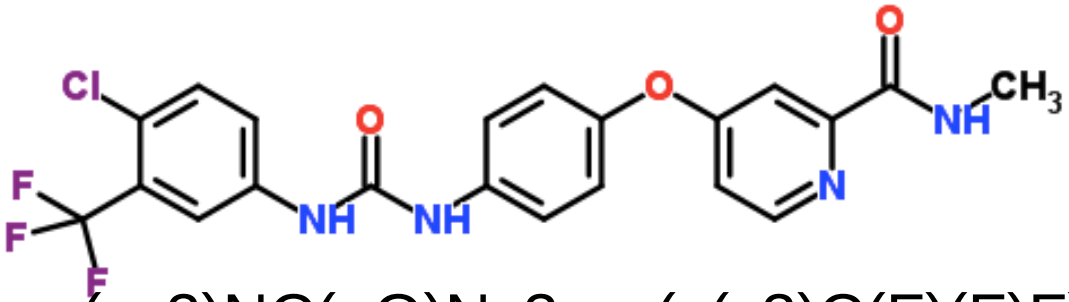
1. More information about a target

https://beta.openphacts.org/target?uri=**http%3A%2F%2Fdata.kasabi.com%2Fdataset%2Fchembl-rdf%2Fchemblid%2FCHEMBL4226**&app_id=0e939a76&app_key=1004d9ef5f4ee1ab0bbfc02b623cb955

Open PHACTS
Open Pharmacological Space

Compound – Target App

Sorafenib
`



SMILIES:
CNC(=O)c1cc(ccn1)Oc2ccc(cc2)NC(=O)Nc3ccc(c(c3)C(F)(F)F)Cl

Dual specificity protein kinase CLK3,

sequence":"MPVLSARRRELADHAGSGRRSGPSPTARSGPHLSALRAQPARAAHLSGRGTYVRRDTAGGGPGQARPLGPPGTSLL
GRGARRSGEGWCPGAFESGARAARPPSRVEPRLATAASREGAGLPRAEVAAGSGRGARSGEWGLAAAGAWETMHHCKRYRSP
EPDPYLSYRWKRRRSYSREHEGRLRYPSRREPPPRRSRSRSHDRLPYQRRYRERRDSDTYRCEERSPSFGEDYYGPSRSRHRR
RSRERGPYRTRKHAHHCHKRRTRSCSSASSRSQQSSKRSSRSVEDDKEGHLVCRIGDWLQERYEIVGNLGEGTFGKVVECLDHA
RGKSQVALKIIRNVGKYREAARLEINVLKKIKEKDKENKFLCVLMSDWFNFHGHMCIAFELLGKNTFEFLKENNFQPYPLPHVRHMAY
QLCHALRFLHENQLTHTDLKPENILFVNSEFETLYNEHKSCEEKSVKNTSIRVADFGSATFDHEHHTTIVATRHYRPPEVILELGWAQP
CDVWSIGCILFEYYRGFTLFQTHENREHLVMMEKILGPIPSHMIHRTRKQKYFYKGGLVWDENSSDGRYVKENCKPLKSYMLQDSLE
HVQLFDLMRRMLEFDPAQRITLAEALLHPFFAGLTPEERSFHTSRNPSR"

GOING FURTHER

More APIs

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Classification APIs

Enzyme Pharmacology Paginated	/target/enzyme/pharmacology/pages	GET
ChEBI Ontology Class Pharmacology Paginated	/compound/chebi/pharmacology/pages	GET

Filtering

Activity types	/pharmacology/filters/activities	GET
Units for activity type	/pharmacology/filters/units/	GET

Client Libraries

Open PHACTS
Open Pharmacological Space

Support for multiple languages
Still in development but useful to get started with
Easy to create libraries

Ruby
- https://github.com/openphacts/ops_gems

Javascript
- https://github.com/openphacts/ops.js

Java
- https://github.com/openphacts/JavaLDAClient

Pipeline Pilot (coming soon)

http://dev.openphacts.org
Create!