
RCSB-API

<https://rcsbapi.readthedocs.io/>

- Rcsb-api Query RCSB PDB data from Python

Pip install rcsb-api

- TextQuery

```
from rcsbapi.search import TextQuery

# Search for structures associated with the phrase "Hemoglobin"
query = TextQuery(value="Hemoglobin")

# Execute the query by running it as a function
results = query()

# Results are returned as an iterator of result identifiers.
for rid in results:
    print(rid)
```

- Attribute search

```
from rcsbapi.search import AttributeQuery

# Construct a query searching for structures from humans
query = AttributeQuery(
    attribute="rcsb_entity_source_organism.scientific_name",
    operator="exact_match", # Other operators include "contains_phrase", "exists", and
    more
    value="Homo sapiens"
)

# Execute query and construct a list from results
results = list(query())
print(results)
```

- Grouping sub-queries

```
from rcsbapi.search import search_attributes as attrs

# Query for human epidermal growth factor receptor (EGFR) structures (UniProt ID P00533)
# with investigational or experimental drugs bound
q1 =
attrs.rcsb_polymer_entity_container_identifiers.reference_sequence_identifiers.database_
accession == "P00533"
q2 = attrs.rcsb_entity_source_organism.scientific_name == "Homo sapiens"
q3 = attrs.drugbank_info.drug_groups == "investigational"
q4 = attrs.drugbank_info.drug_groups == "experimental"

# Structures matching UniProt ID P00533 AND from humans
# AND (investigational OR experimental drug group)
query = q1 & q2 & (q3 | q4)

# Execute query and print first 10 ids
results = list(query())
print(results[:10])
```

-Supported Search Services

Search service

QueryType

Full-text

`TextQuery()`

Attribute (structure or chemical)

`AttributeQuery()`

Sequence similarity

`SeqSimilarityQuery()`

Sequence motif

`SeqMotifQuery()`

Structure similarity

`StructSimilarityQuery()`

Structure motif

`StructMotifQuery()`

Chemical similarity

`ChemSimilarityQuery()`

<https://search.rcsb.org/#search-services>

<https://github.com/rcsb/py-rcsb-api/tree/master/notebooks>