

REST API

introduction

State

- Simple REST API is available
- Molecules, descriptors are represented
- Molecules can be accessed
- Similarity search for molecule targets can be invoked
- Client web page example for invoking similarity search is available

Querying descriptors

Invoke similarity search:

```
/rest/descriptors/zinc-all-cfp7/find-most-similarers?&count=10&w=400&h=400&query=CCC
```

Parameters:

- **Descriptor ID** identifies a specific fingerprint (associated with a set of molecules). Multiple fingerprints for multiple molecule sets can be stored
- **Target image dimensions** The response will contain URL to acquire the targets as images. Image dimensions for this URL can be specified
- **Query structure** as SMILES string
- **Number** of the most similar targets to return

Response JSON

```
{ "searchtime" : 85,  
  "query"      : "CCC" ,  
  "querysmi"  : "CCC",  
  "targets": [  
    { "dissimilarity" : 0.0,  
      "targetindex"  : 806176,  
      "targetid"     : "ZINC02040556",  
      "targetmolurl" : "rest/molecules/zinc-all/806176",  
      "targetimageurl" : "rest/molecules/zinc-all/806176/png?w=400&h=400",  
      "base64img"    : null  
    } , { ... } , { ... } , ... , { ... }  
  ]  
}
```

- Multiple target count can be requested
- Index of the target structure
- Target ID imported from the structure file
- URL of target structure image
- Target structure image can be requested as base64 encoded png

Further information

- REST API documentation generated by enunciate
- HTML usage example

Example CLI usage

Import molecules and molecule names as ID

```
createMms -in vitamins.smi \  
-name data/vitamins-name.bin \  
-out data/vitamins-mms.bin
```

Calculate CFP-7 fingerprint

```
buildStorage -context createSimpleCfp7Context \  
-in vitamins.smi \  
-out data/vitamins-cfp7.bin
```

Launch embedded server; specify molecules and fingerprints to expose

```
gui -nobrowse  
-mols -name:vitamins:-mms:data/vitamins-mms.bin:-mid:data/vitamins-name.bin \  
-desc -desc:data/vitamins-cfp7.bin:-mols:vitamins:-name:vita-cfp7 \
```

Input structures

Binary file for structure ID

Binary file for structures

Binary file for fingerprints

REST resource associated to the structures

REST resource associated to this fingerprint